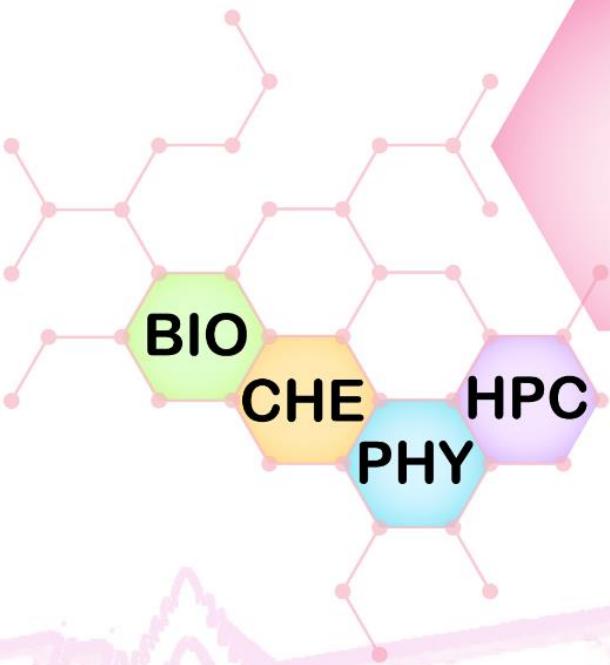
The 22nd International Annual Symposium on Computational Science and Engineering



Faculty of Science, Chulalongkorn University
Bangkok, Thailand
Aug 2-3, 2018

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WELCOME MESSAGE

On behalf of the Faculty of Science, Chulalongkorn University, I am truly honored and delighted to welcome you to the 22nd International Annual Symposium on Computational Science and Engineering (ANSCSE22). This year the conference is being held during August 2-3, 2018 at Faculty of Science, Chulalongkorn University, Bangkok, Thailand. This conference covers issues on Computational Biology, Chemistry, Physics, Mathematics and High-Performance Computing. I do hope that ANSCSE22 will be a platform to create a stage for exchanging the latest research results and sharing the advanced research ideas about all aspects of Computational Science and Engineering.

As the third largest faculty of the university, we are proud to be one of the best academic and intellectual institution in nation. The Faculty of Science also commits to provide professional services in the form of research consultation, workshops, seminars, national and international conferences, technology transfer and development. Therefore, we are pleased to have the opportunity to host for this event.

I would like to express my gratitude to the conference organizing committee, sponsors, technical support staffs, and participants who make this event remarkably successful. With your participation, I do believe that this conference will result in future collaborations between universities and research institutions both locally and internationally.

I wish all the success for this conference, and I also wish all of you taken an extra time to enjoy the spectacular and unique beauty of Thailand.

With best wishes,

Polkit Sangvanich

(Professor Dr. Polkit Sangvanich)
Dean, Faculty of Science,
Chulalongkorn university

WELCOME MESSAGE

The 22nd session of the International Annual Symposium on Computational Science and Engineering or ANSCSE 22is hosted by Faculty of Science, Chulalongkorn University. This long continuation of the symposium cannot at all be realized without strong support from host institutions. It also suggested that the community of computational scientists is very well established in Thailand. Usually, there are four parallel sessions with six areas of research. They included computational chemistry, computational biology, computational physics and fluid dynamics, and computer science and high-performance computing. In the future, we might need to include "data science" as one of the research areas, since it is the today growing field. For this year, I would like to thank Chulalongkorn University, the host, for their willingness and consistent effort in putting a tremendous scientific program. This is not the first time that they hosted this event, but the third time. Also, thanks go to our plenary lecturers, Professor David Ruffolo from Mahidol University, Professor Putchong Uthayopas from Kasetsart University, and Professor Ras B. Pandey from University of Southern Mississippi, U.S.A. Last but not least, thanks to our invited speakers and all participants of ANSCSE 22. I hope you all will continue to join and support this annual symposium for the next year.

Associate Professor Dr. Vudhichai Parasuk
President of Computational Science and Engineering Association (CSEA)

WELCOME MESSAGE

On behalf of the organizing committee, I am honored and delighted to welcome you to the 22nd International Annual Symposium on Computational Science and Engineering (ANSCSE22) at Faculty of Science, Chulalongkorn University.

As a conference chair, I know that the success of the conference depends ultimately on the many people who have worked with us in planning and organizing both the scientific program and supporting arrangements. In particular, we thank the Program Chairs for organizing the technical program, the Program Committee for their thorough and timely reviewing of the papers, our sponsors who have helped us to keep down the costs of ANSCSE22, and all participants who contribute to the progress of scientific research in their field. Recognition should go to the Organizing Committee members who have all worked extremely hard for the details of important aspects of the conference programs and activities.

Professor Dr. Supot Hannongbua
Conference Chair of ANSCSE22

COMMITTEE

Steering Committee

Asst. Prof. Putchong Uthayopas, Kasetsart University, Thailand

Assoc. Prof. Vudhichai Parasuk, Chulalongkorn University and Acting President of CSEA, Thailand

Prof. Supa Hannongbua, Kasetsart University, Thailand

Honorary Chair

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Assoc. Prof. Vejapong Juttijudata, Kasetsart University, Thailand

Asst. Prof. Putchong Uthayopas, Kasetsart University, Thailand

Assoc. Prof. Vara Varavithya, King Mongkut's University of Technology North Bangkok, Thailand

Dr. Supakit Prueksaaroon, Thammasat University, Thailand

Dr. Supawadee Namuangruk, National Nanotechnology Center (NANOTEC), NSTDA, Thailand

COMMITTEE

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Assoc. Prof. Norio Yoshida, Kyoshu University, Japan

Prof. Seiji Mori, Ibaraki University, Japan

Assoc. Prof. Hisashi Okumura, Institute for Molecular Science, Japan

Prof. Jen-Shiang K. Yu, National Chiao Tung University, Taiwan

Dr. Kaito Tankahashi, Academia Sinica, Taiwan

Prof. Ras B. Pandey, University of Southern Mississippi, USA

Prof. Eduardo Perozo, University of Chicago, USA

Prof. Michael Green, City College of the City University of New York, USA

Organizing Committee Chair

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Dr. Nattapong Paiboonvorachat, Chulalongkorn University, Thailand

Asst. Prof. Thanyada Rungrotmongkol, Chulalongkorn University, Thailand

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GENERAL INFORMATION

Conference Venue
Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

Registration
Registration desk is located in front of the conference room 207 on the 2nd floor of MHMK building.

Registration hours:	Thursday, 2nd August	8:00 - 16:00
	Friday, 3rd August	8:00 - 12:00

Badges
Badges can be picked up on 2nd-3rd August at the registration desk and should be worn for admission to all scientific sessions and the social events.

Workshop
The workshop will take place in 1101/2 Self-Learning Room (Chemistry Library), The 11th floor, MHMK building on Wednesday, 1st August.

Conference Rooms
The conference rooms are 205, 206, 207 and 208 on the 2nd floor of MHMK building.

Plenary and Invited Speakers, Oral Presenters
We kindly ask all speakers to come to the conference room to load/check their presentation at least **20 minutes** prior to their session to ensure the presentation is checked and tested. Technical staffs in the room will assist in uploading and setting up your presentation. Presentations should be provided in a version of Microsoft PowerPoint. If your presentation is in MAC format, it is imperative that this be converted to PC format. Please make a copy of your presentation in your flash drive in order to upload onsite. If speakers wish to use their own laptop, please inform the staff prior to the start of your session for setting up your laptop with the projector.

Poster Session
Poster session is located on the 3rd floor of MHMK building. The poster boards can fit posters up to the A0 size (Width x Height : 84.1 × 118.9 cm, or 33.1 in × 46.8 in) in portrait orientation. Printed posters should be mounted beginning at 8:00 on Thursday 2nd Aug and MUST be removed by 18:00 on the same day. Posters are arranged according to research areas. Posters with an odd ID number should be presented from 13:55-14:45. Posters with an even ID number should be presented from 14:45-15:35. For e-Poster, there will be either laptop or TV monitor provided.

Internet Access
To access internet, Chulalongkorn University wireless is available free-of-charge. Please contact IT Staff for internet access account and code.

GENERAL INFORMATION

Lunch
Lunch will be served at the ground floor of MHMK building.

Exhibition
The exhibition is located at the 2nd floor of MHMK building. The “Vendor Session” will be held on 2nd August, 15:45-17:20 at room 206.

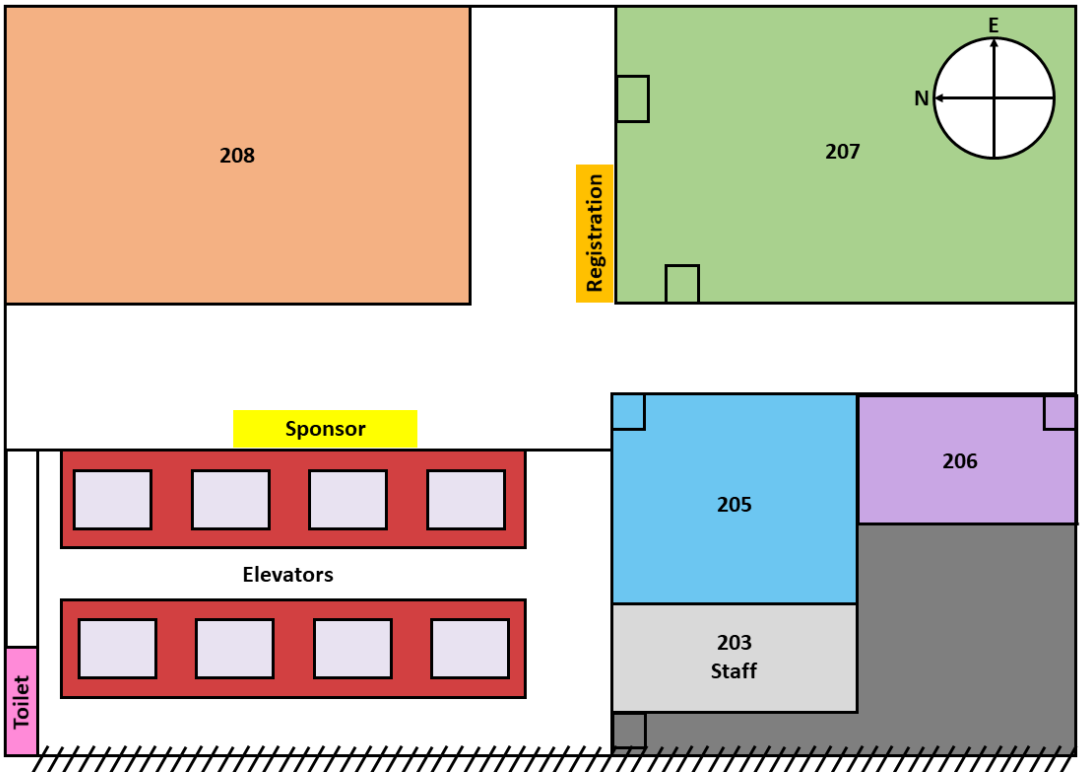
Banquet
The banquet will take place on 2nd August at Ho Noy, the ground floor of Poonsub Nopphawong Na Ayutthaya Building, Faculty of Education.

CU Shuttle Bus
Chulalongkorn University provides free shuttle service for faculty, staff, students, and visitors with safe and convenient transportation to most sites on campus. The shuttle service runs during from Monday to Saturday, 7AM – 7PM.
For more details please visit the website: https://www.chula.ac.th/en/about/green-university/cu-shuttle-bus/

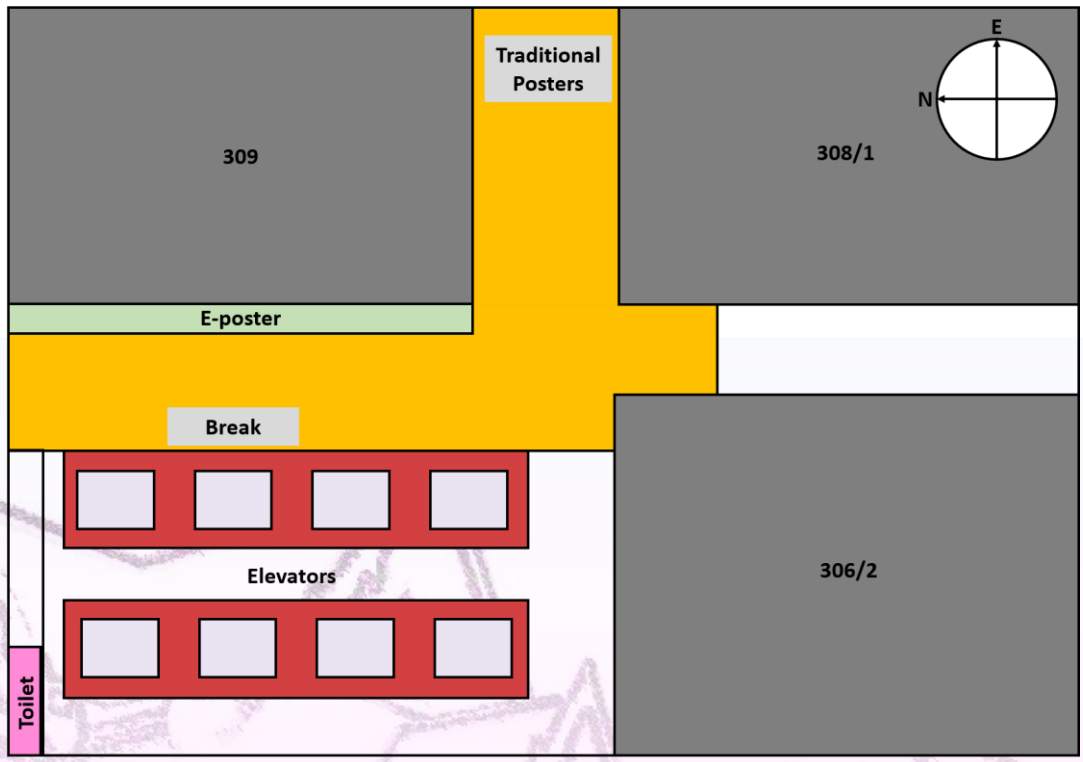
MAP

CONFERENCE ROOM

2nd floor MHMK Building

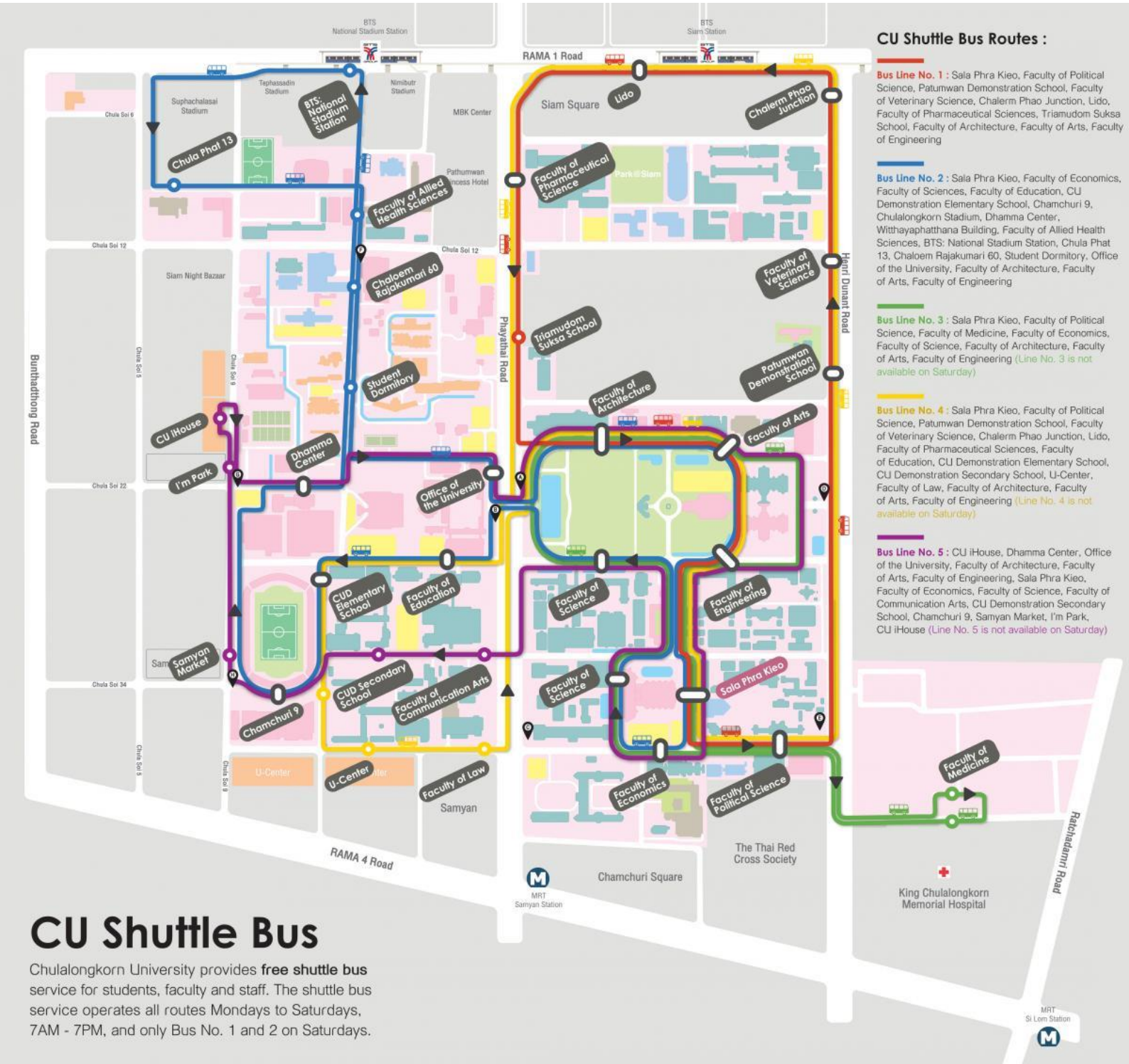


3rd floor MHMK Building



MAP

Chulalongkorn University map link to public transportation



CU Shuttle Bus

Chulalongkorn University provides **free shuttle bus** service for students, faculty and staff. The shuttle bus service operates all routes Mondays to Saturdays, 7AM - 7PM, and only Bus No. 1 and 2 on Saturdays.

MAP

BANQUET LOCATION

PLENARY LECTURE

PL-1: Monte Carlo simulations of energetic particle transport in space, in Earth's atmosphere, and in a cosmic ray detector

David Ruffolo

Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand

PL-2: Future of High Performance Computing

Putchong Uthayopas

Department of Computer Engineering, Faculty of Engineering,
Kasetsart University, Bangkok, Thailand

PL-3: Morphing structures and dynamics by a multigrain approach

Ras B. Pandey

Department of Physics and Astronomy
University of Southern Mississippi, Hattiesburg, USA

LIST OF INVITED SPEAKERS

Computational Biology, Bioinformatics, Biochemistry and Biophysics

BIO-INV-01	Yasuteru	Shigeta	University of Tsukuba	Japan
BIO-INV-02	Hisashi	Okumura	Institute for Molecular Science	Japan
BIO-INV-03	Satoru G.	Itoh	Institute for Molecular Science	Japan
BIO-INV-04	Michael E	Green	The City College of CUNY	USA
BIO-INV-05	Norio	Yoshida	Kyushu University	Japan
BIO-INV-06	Chia-Ching	Chang	National Chiao Tung University	Taiwan
BIO-INV-07	Tawun	Remsungnen	Khon Kaen University	Thailand
BIO-INV-08	Jen-Shiang K.	Yu	National Chiao Tung University	Taiwan
BIO-INV-09	Sira	Sriswasdi	Chulalongkorn University	Thailand
BIO-INV-10	Chih-Hao	Lu	China Medical University	Taiwan

Computational Chemistry

CHE-INV-01	Seiji	Mori	Ibaraki University	Japan
CHE-INV-02	Tanin	Nanok	Kasetsart University	Thailand
CHE-INV-03	Phornphimon	Maitarad	Shanghai University	China
CHE-INV-04	Kaito	Takahash	Academia Sinica	Taiwan
CHE-INV-05	Pussana	Hirunsit	NANOTEC, NSTDA	Thailand
CHE-INV-06	Paul M.	Gleeson	KMITL	Thailand
CHE-INV-07	Deva U.	Priyakumar	International Institute of Information Technology	India
CHE-INV-08	Thana	Maihom	Kasetsart University	Thailand
CHE-INV-09	Tatiya	Chokbunpiam	Ramkhamhaeng University	Thailand

LIST OF INVITED SPEAKERS

Computational Fluid Dynamics and Solid Mechanics

PHY-INV-01	Pakpoom	Reunchan	Kasetsart University	Thailand
PHY-INV-02	Jariyanee	Prasongkit	Nakhon Phanom University	Thailand
PHY-INV-03	Thanayut	Kaewmaraya	Khon Kaen University	Thailand
PHY-INV-04	Udomsilp	Pinsook	Chulalongkorn University	Thailand
PHY-INV-05	Rob	Knoops	Chulalongkorn University	Thailand
PHY-INV-06	Adisak	Boonchun	Kasetsart University	Thailand
PHY-INV-07	Worasak	Sukkabot	Ubon Ratchathani University	Thailand

High Performance Computing, Computer Science, Mathematics and Engineering

HPC-INV-01	Rudklao	Pan-Aram	Electricity Generating Authority of Thailand	Thailand
HPC-INV-02	Monrudee	Liangruksa	NANOTEC	Thailand
HPC-INV-03	Manaschai	Kunaseth	NANOTEC, NSTDA	Thailand
HPC-INV-04	Thiansin	Liamsuwan	Chulabhorn Royal Academy	Thailand

PROGRAMME

Wednesday, 1st August 2018

Location: Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University

Workshop

Time		Room
08:30-09:00	Registration for Workshop (11th Floor)	1101/2 Self-Learning Room (Chemistry Library) 11th Floor
09:00-12:00 (Lecture)	Workshop: Ab Initio Simulation of Reaction Rates and Vibrational Spectra Professor Dr. Kaito Takahashi, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan	
13:00-16:00 (Practice)	Demonstration	

PROGRAMME

Thursday, 2nd August 2018

Location: Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University

Conference Day 1

Time				Room
08:00-08:30	Registration			2nd Floor
08:30-08:45	Opening Ceremony Professor Dr. Polkit Sangvanich, Dean of Faculty of Science			207 2nd Floor
08:45-09:30	Plenary Lecture 1 Title: Monte Carlo simulations of energetic particle transport in space, in Earth's atmosphere, and in a cosmic ray detector Professor Dr. David Ruffolo. Department of Physics, Mahidol University			
09:30-09:40	Group Photo			
09:40-10:00	Coffee Break			2nd Floor
Oral Presentation 1 (Parallel Sessions)				
Session	Room 208	Room 207	Room 205	Room 206
	BIO 1	CHE 1	PHY 1	HPC 1
10:00-12:00	BIO-INV-01 BIO-INV-02 BIO-INV-03	CHE-INV-01 CHE-INV-02 CHE-INV-03	PHY-INV-01 PHY-INV-02 PHY-INV-03	HPC-INV-01 HPC-INV-02
	BIO-ORA-01e BIO-ORA-02e BIO-ORA-03t	CHE-ORA-01t CHE-ORA-02t CHE-ORA-03e	PHY-ORA-01 PHY-ORA-02e PHY-ORA-03t	HPC-ORA-01e HPC-ORA-02e HPC-ORA-03e
12:00-13:00	Lunch			Ground Floor
13:00-13:45	Plenary Lecture 2 Title: Future of High Performance Computing Assistant Professor Dr. Putchong Uthayopas, Department of Computer Engineering, Kasetsart University			207 2nd Floor
13:50-15:40	Poster Session Odd-numbered poster: 13.55-14.45 Even-numbered poster: 14.45-15.35			3rd Floor
	Coffee Break (Starting at 14:30 on the 3rd floor)			
Oral Presentation 2 (Parallel Sessions)				
Session	Room 208	Room 207	Room 205	Room 206
	BIO 2	CHE 2	PHY 2	Special Session
15:45-17:20	BIO-INV-04 BIO-INV-05	CHE-INV-04 CHE-INV-05	PHY-INV-04 PHY-INV-05	Hewlett Packard Enterprise | intel
	BIO-ORA-04e BIO-ORA-05t BIO-ORA-06t	CHE-ORA-04t CHE-ORA-05t CHE-ORA-06	PHY-ORA-04t PHY-ORA-05e PHY-ORA-06e	DELL EMC
18:00-20:00	Banquet Location: Ho Noy, Poonsub Nopphawong Na Ayutthaya Building (Ground Floor), Faculty of Education			

PROGRAMME

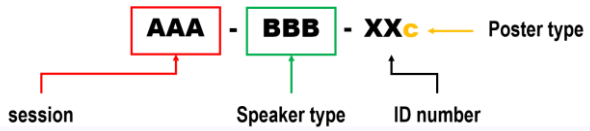
Friday, 3rd August 2018

Location: Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University

Conference Day 2

Time				Room
08:00-09:00	Registration			2nd Floor
09:00-09:45	Plenary Lecture 3 Title: Morphing Structures and Dynamics by Multi-Grain Computer Simulation Modeling Professor Dr. Ras B. Pandey, University of Southern Mississippi, USA			207 2nd Floor
09:45-10:00	Coffee Break			2nd Floor
Oral Presentation 3 (Parallel Sessions)				
Session	Room 208	Room 207	Room 205	Room 206
	BIO 3	CHE 3	PHY 3	HPC 2
10:00-11:45	BIO-INV-06 BIO-INV-07 BIO-INV-08	CHE-INV-06 CHE-INV-07	PHY-INV-06 PHY-INV-07	HPC-INV-03 HPC-INV-04
	BIO-ORA-07e BIO-ORA-08e	CHE-ORA-07t CHE-ORA-08	PHY-ORA-07e PHY-ORA-08	HPC-ORA-04 HPC-ORA-05e
11:45-13:00	Lunch			Ground Floor
Oral Presentation 4 (Parallel Sessions)				
Session	Room 208	Room 207	Room 205	
	BIO 4	CHE 4	CHE 5	
13:00-14:05	BIO-INV-09 BIO-INV-10 BIO-ORA-09e	CHE-INV-08 CHE-ORA-09e CHE-ORA-10e	CHE-INV-09 CHE-ORA-11 CHE-ORA-12e	
14:30-15:00	Presentation Awards & Closing & Rich Coffee			207

Presentation Code Definition



AAA: BIO = Computational Biology, Bioinformatics, Biochemistry and Biophysics
CHE = Computational Chemistry
PHY = Computational Physics, Computational Fluid Dynamics and Solid Mechanics
HPC = High Performance Computing, Computer Science, Mathematics and Engineering

BBB: INV = Invited Speaker
ORA = Oral Presenter
POS = Poster Presenter

XX: ID number

c: The letter indicates the presenter who is going to present their work in both ORAL and POSTER sessions.
Poster type is indicated as following:
t = Paper printed poster
e = E-poster

PROGRAMME

Thursday, 2nd August 2018

Location: Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University

Room 207, MHMK Building, Time 8:00-10:00

Time	
08:00-08:30	Registration
08:30-08:45	Opening Ceremony Welcome Remarks Professor Polkit Sangvanich, Dean of Faculty of Science MC: *Thanyada Rungrotmongkol and Tanin Nanok*
08:45-09:30	Plenary Lecture 1 Professor Dr. David Ruffolo. Department of Physics, Mahidol University Title: Monte Carlo simulations of energetic particle transport in space, in Earth's atmosphere, and in a cosmic ray detector *Chair: Supot Hannongbua, Chulalongkorn University*
09:30-09:40	Group Photo
09:40-10:00	Coffee Break

Room 207, MHMK Building

Time	
13:00-13:45	Plenary Lecture 2 Assistant Professor Dr. Putchong Uthayopas, Department of Computer Engineering, Faculty of Engineering, Kasetsart University Title: Future of High Performance Computing *Chair: Supa Hannongbua, Kasetsart University*

PROGRAMME

Thursday, 2nd August 2018

Computational Biology, Bioinformatics, Biochemistry and Biophysics

Session BIO 1
Co-chairs : *Yasuteru Shigeta, University of Tsukuba*
Hisashi Okumura, Institute for Molecular Science

Room 208, MHMK Building
Time 10:00-12:00

Time	Code	Presenter	Title
10:00-10:25	BIO-INV-01	Yasuteru Shigeta University of Tsukuba, Japan	Data-driven Parallel Cascade Selection Molecular Dynamics
10:25-10:50	BIO-INV-02	Hisashi Okumura Institute for Molecular Science, Japan	Simulational studies of Aβ amyloid fibrils by molecular dynamics method
10:50-11:15	BIO-INV-03	Satoru Itoh Institute for Molecular Science, Japan	Molecular dynamics simulations of a full-length amyloid-β peptide at a hydrophobic/hydrophilic interface
11:15-11:30	BIO-ORA-01e	Panupong Mahalapbutr Chulalongkorn University	Anticancer activity of mansonone G derivatives against human non-small cell lung cancer
11:30-11:45	BIO-ORA-02e	Bodee Nutho Chulalongkorn University	Reaction Mechanism of the Zika Virus NS2B/NS3 Serine Protease with Its Substrate: A QM/MM Study
11:45-12:00	BIO-ORA-03t	Wansiri Innok Thaksin University	The Potential of Interested Leading Alkaloid and Flavonoid Compounds in Thai Herbs against Achetylcholinesterase Inhibitory of Alzheimer's Disease

Session BIO 2
Co-chairs : Michael Green, CCNY
: Norio Yoshida, Kyoshu University

Room 208, MHMK Building
Time 15:45-17:20

Time	Code	Presenter	Title
15:45-16:10	BIO-INV-04	Michael Green City College of the City University of New York, USA	Quantum Calculations on the Voltage Sensing Domain of a Voltage Gated Ion Channel
16:10-16:35	BIO-INV-05	Norio Yoshida Kyoshu University, Japan	Theoretical study of biological processes employing statistical mechanics of molecular liquids
16:35-16:50	BIO-ORA-04e	Phakawat Chusuth Chulalongkorn University	The binding of cobratoxin from Naja kaouthia towards nicotinic acetylcholine receptor (nAChR)
16:50-17:05	BIO-ORA-05t	Tadsanee Awang Kasetsart University	Computational studies of the adsorption of human defensin 5 on bacterial membranes
17:05-17:20	BIO-ORA-06t	Channarong Khrutto Chulalongkorn University	Molecular dynamics simulations of M2 channel in phospholipid bilayers with different thickness

PROGRAMME

Thursday, 2nd August 2018

Computational Chemistry

Session CHE 1
Co-chairs: *Kaito Takahashi, Academia Sinica*
: *Supawadee Namungruk, NSTDA*

Room 207, MHMK Building
Time 10:00-12:00

Time	Code	Presenter	Title
10:00-10:25	CHE-INV-01	Seiji Mori Ibaraki University, Japan	Mechanistic Insights into Metal-Catalyzed Highly Selective Organic Transformation Reactions
10:25-10:50	CHE-INV-02:	Tanin Nanok Kasetsart Unversity	Towards a Molecular Understanding of the Relative Reactivities of ε-Caprolactone and L-Lactide in Their Homo- and Copolymerization Using Aluminium Salen-type Initiators: A DFT Study Screen reader support enabled
10:50-11:15	CHE-INV-03	Phornphimon Maitarad, Shanghai University, China	QSAR Study of Phenoxy-imine Catalytic Behavior in Polyethylene Polymerization
11:15-11:30	CHE-ORA-01t	Nuttaporn Janprapa King Mongkut's University of Technology Thonburi	A theoretical study of fluorene based copolymers for solar cell applications
11:30-11:45	CHE-ORA-02t	Rattanawalee Rattanawan Ubon Ratchathani University	Molecular Engineering of D-A Featured Organic Indole Sensitizers for Improving Performance Efficiency of Dye-Sensitized Solar Cells
11:45-12:00	CHE-ORA-03e	Pipat Khongpracha Kasetsart University	Charge Carriers Distribution in Platinum Doped Graphitic Carbon Nitride Quantum Dot

Session CHE 2
Cc-chairs: *Deva Priyakumar, IIIT Hyderabad*
: Pussana Hirunsit, NSTDA

Room 207, MHMK Building
Time 15:45-17:20

Time	Code	Presenter	Title
15:45-16:10	CHE-INV-04	Kaito Takahashi Academia Sinica, Taiwan	The Imprint of Electronic Structure on the Reactivity of Linear Carbon Chain Cations
16:10-16:35	CHE-INV-05	Pussana Hirunsit NANOTEC, NSTDA	Theoretical Investigation of CO_2 Electrochemical Reduction on Cu-based Catalysts: The Effect of Surface Facets and The Role of S Dopant
16:35-16:50	CHE-ORA-04t	Yuwanda Injongkol Ubon Ratchathani University	The mechanism of carbon dioxide hydrogenation to formic acid on Pt-boron nitride nanosheets (Pt-BNNSs): A theoretical study
16:50-17:05	CHE-ORA-05t	Nuttapon Yodsin Ubon Ratchathani University	The theoretical study of catalytic CO2 hydrogenation to formic acid over a metal-decorated carbon nanocone
17:05-17:20	CHE-ORA-06	Preeyaporn Poldorn Ubon Ratchathani University	Ag7Au6 cluster as a highly active catalyst for CO oxidation: Theoretical study

PROGRAMME

Thursday, 2nd August 2018

Computational Physics, Fluid Dynamic and Solid Mechanics

Session PHY 1
Co-chairs: *Thanayut Kaewmaraya, Khon Kaen University*
: *Pakpoom Reunchan, Kasetsart University*

Room 205, MHMK Building
Time 10:00-12:00

Time	Code	Presenter	Title
10:00-10:25	PHY-INV-01	Pakpoom Reunchan Kasetsart University	Self-trapped hole in BaTiO3
10:25-10:50	PHY-INV-02	Jariyanee Prasongkit Nakhon Phanom University	First-Principles Study of Two-Dimensional Materials for Nanoelectronics
10:50-11:15	PHY-INV-03	Thanayut Kaewmaraya Khon Kaen University	2D van der Waals Heterostructures for Nanoelectronics
11:15-11:30	PHY-ORA-01	Sujin Suwanna Mahidol University	First-Principle Study of Strain-Induced Band Gap Tunability of Two-Dimensional Transition Metal Dichalcogenides MX2 (M = Mo, W; X = O, S, Se, Te)
11:30-11:45	PHY-ORA-02e	Abdulmutta Thatribud Prince of Songkla University	Electronic and Optical Properties of Silver Chloride Photocatalyst by First Principles calculation
11:45-12:00	PHY-ORA-03t	Sorayot Chinkanjanarot National Metal and Materials Technology Center	Predicting Coefficient of Linear Thermal Expansion of Carbon Fiber/Graphene Nanoplatelet/EPON862 Hybrid Composites: Multiscale Modeling

Session PHY 2
Co-chairs: *Rob Knoops, Chulalongkorn University*
: *Udomsilp Pinsook, Chulalongkorn University*

Room 205, MHMK Building
Time 15:45-17:20

Time	Code	Presenter	Title
15:45-16:10	PHY-INV-04	Udomsilp Pinsook Chulalongkorn University	Essence of Correlation Energy
16:10-16:35	PHY-INV-05	Rob Knoops Chulalongkorn University	Inflation from Supersymmetry Breaking
16:35-16:50	PHY-ORA-04t	Somboon Otarawanna National Metal and Materials Technology Center	Matrix Tridiagonalization Methods for 3D Finite Element Analysis of Free Vibration
16:50-17:05	PHY-ORA-05e	Wanfeng Yu Mae Fah Luang University	Identify Transient Sources from GOTO Sky Survey Data with Clustering Method
17:05-17:20	PHY-ORA-06e	Vichayanun Wachirapusitanand Chulalongkorn University	Machine Learning system mimicking student's choice in Particle Data Analysis laboratory activity

PROGRAMME

Thursday, 2nd August 2018

High Performance Computing, Computer Science, Mathematic & Engineering

Session HPC 1 Co-chairs: :			Room 206, MHMK Building Time 10:00-11:35
Time	**Code**	**Presenter**	**Title**
10:00-10:25	HPC-INV-01	Rudklao Panaram Electricity Generating Authority of Thailand	Mathematics Computing in Environmental Quality for Power Plant
10:25-10:50	HPC-INV-02	Monrudee Liangruksa National Nanotechnology Center, Thailand	Mathematical modeling and analysis of thermal transport for materials design
10:50-11:05	HPC-ORA-01e	Piyakorn Phanklin Thammasat University	Loop prevention on Software Defined Network using Adaptive Virtual Tunnel Network
11:05-11:20	HPC-ORA-02e	Kanjanart Junnawat Thammasat University	Resilience flow management on Software-Defined Network using Directed graph for L2 Loop prevention
11:20-11:35	HPC-ORA-03e	Dussadee Somjaiwang King Mongkut's University	Existence and Approximation of Solutions of Coupled Fractional Order Hybrid Differential Equations

PROGRAMME

Thursday, 2nd August 2018

Special Vendor Session

			Room 206, MHMK Building **Time 15:45-17:15**
Time	**Code**	**Presenter**	**Title**
15:45-16:30	-	Hewlett Packard Enterprise / intel	**HPE Enterprise Infrastructure for HPC / AI / Deep Learning**
16:30-17:15	-	DELL EMC	**Providing AI and ML Technology That Makes Tomorrow possible, Today**

Note: Presentation in Thai

PROGRAMME

Friday, 3rd August 2018

Location: Mahamakut (MHMK) Building, Faculty of Science, Chulalongkorn University

Room 207, MHMK Building

Time	
09:00-09:45	Plenary Lecture 3 **Professor Ras B. Pandey, University of Southern Mississippi, USA** **Title: Morphing structures and dynamics by multi-grain computer simulation modeling** Chair: ***Siriporn Jungsutiwong, Ubon Ratchathani University***

Friday, 3rd August 2018

Computational Biology, Bioinformatics, Biochemistry and Biophysics

Session BIO 3
Co-chairs: *Chia-Ching Chang, National Chiao Tung University*
: *Chih-Hao Lu, China Medical University*

Room 208, MHMK Building
Time 10:00-11:45

Time	Code	Presenter	Title
10:00-10:25	BIO-INV-06	Chia-Ching Chang National Chiao Tung University, Taiwan	Structure and conducting mechanism characterization of DNA template guided nickel ion chain
10:25-10:50	BIO-INV-07	Tawun remsungnen Khon Kaen University	Biocompatible MOFs for Drug Delivery: Computational Studies
10:50-11:15	BIO-INV-08	Jen-Shiang K. Yu National Chiao Tung University, Taiwan	Catalytic Roles of Histidine and Arginine in Pyruvate Class II Aldolase
11:15-11:30	BIO-ORA-07e	Kanyani sangpheak Chulalongkorn University	In silico and in vitro studies of chalcones as potent anticancer agents with EGFR kinase
11:30-11:45	BIO-ORA-08e	Kanika Verma Chulalongkorn University	Exploring the Impact of R306C and F270V Mutations in β-Tubulin Structure and Function: A Computational Perspective

Session BIO 4
Ci-chairs: *Jen-Shiang K. Yu, National Chiao Tung University*

Room 208, MHMK Building
Time 13:00-14:05

Time	Code	Presenter	Title
13:00-13:25	BIO-INV-09	Sira Sriswasdi Faculty of Medicine, Chulalongkorn University	Toward Next-Generation Neoantigen Prediction with Deep Learning
13:25-13:50	BIO-INV-10	Chih-Hao Lu China Medical University, Taiwan	The relationship between protein function and local structural conservation
13:50-14:05	BIO-ORA-09e	Thapanar Suwanmajo Chiang Mai University	Tunable Signal Processing in Multi-site Phosphorylation Systems via Explicit Enzyme Activation

PROGRAMME

Friday, 3rd August 2018

Computational Chemistry

Session CHE 3
Co-chairs: *Seiji Mori, Ibaraki University*
: Phornphimon Maitarad, Shanghai University
Room 207, MHMK Building
Time 10:00-11:20

Time	Code	Presenter	Title
10:00-10:25	CHE-INV-06	Matthew Paul Gleeson King Mongkut's Institute of Technology	Application of Computational Methods in Anti-malarial Drug Discovery
10:25-10:50	CHE-INV-07	Deva Priyakumar International Institute of Information Technology, Hyderabad, India	Significance of Urea-Aromatic Interactions in Biology: A Computational Study
10:50-11:05	CHE-ORA-07t	Panyakorn Taweechat* Chulalongkorn University	Molecular dynamics simulations of hyaluronic acid in water
11:05-11:20	CHE-ORA-08	Chartniwat Suksamrarn Kasetsart University	Computational Study of Binding Mode of Depsidones in Vascular Endothelial Growth Factor Receptor-2

Session CHE 4
Chair: *Siriporn Jungsutiwong, Ubon Ratchathani University*
Room 207, MHMK Building
Time 13:00-13:55

Time	Code	Presenter	Title
13:00-13:25	CHE-INV-08	Thana Maihom Kasetsart University Kamphaeng Saen Campus	Designing Efficient Nanoporous Catalysts for Industrial Chemical Reactions
13:25-13:40	CHE-ORA-10e	Wasut Pornpatcharapong Chiang Mai University	Efficient Two-dimensional Ion Pairing Free Energy Surface Computation with Gaussian Process Regression
13:40-13:55	CHE-ORA-09e	Wiparat Hotarat Chulalongkorn University	Delivery of Alpha-mangostin through biological membrane using cyclodextrins: A molecular dynamics simulation study

Session CHE 5
Chair: *Tatiya Chokbunpiam, Ramkhamhaeng University*
Room 205, MHMK Building
Time 13:00-13:55

Time	Code	Presenter	Title
13:00-13:25	CHE-INV-09	Tatiya Chokbunpiam Ramkhamhaeng University	Temperature and Gas Loading Induced Structural-Dynamics Properties of Zeolitic Imidazolate Framework-90
13:25-13:40	CHE-ORA-11	Jitrayut Jitonnom Demonstration School of University of Phayao	Computational Modeling of Cationic Metallocene Polymerizations of 2-Oxazoline
13:40-13:55	CHE-ORA-12e	Cangtao Yin Institute of Atomic and Molecular Sciences, Academia Sinica	The reaction between Criegee intermediates and sulfur dioxide: not really barrierless

PROGRAMME

Friday, 3rd August 2018

Computational Physics, Fluid Dynamic and Solid Mechanics

Session PHY 3 Co-chairs: *Worasak Sukkabot, Ubon Ratchathani University* : *Adisak Boonchun, Kasetsart University*			Room 205, MHMK Building Time 10:00-12:00
Time	**Code**	**Presenter**	**Title**
10:00-10:25	PHY-INV-06	Adisak Boonchun Kasetsart University	The response of electronic properties of monolayer to elastic strain and the stacking stability of bilayer C2N
10:25-10:50	PHY-INV-07	Worasak Sukkabot Ubon Ratchathani University	Atomistic tight-binding theory in alloy semiconductor nanostructures
10:50-11:05	PHY-ORA-07e	Maneerat Chotsawat Synchrotron Light Research Institute	First-principles study of defects in Bi and Al doped orthorhombic PbZrO3
11:05-11:20	PHY-ORA-08	Wutthikrai Busayaporn Synchrotron Light Research Institute	Surface Structure Determination of TiO2(110)(1x2) Dynamic Scattering of Electrons in LEED-IV

PROGRAMME

Friday, 3rd August 2018

High Performance Computing, Computer Science, Mathematic & Engineering

Session HPC 2 Co-chairs: :			Room 206, MHMK Building Time 10:00-11:20
Time	**Code**	**Presenter**	**Title**
10:00-10:25	HPC-INV-03	Manaschai Kunaseth National Nanotechnology Center, Thailand	Shift/Collapse Algorithm for Fast and Scalable Many-Body n-Tuple Computation on Supercomputers
10:25-10:50	HPC-INV-04	Thiansin Liamsuwan Thailand Institute of Nuclear Technology	Computational Approaches for Pre-Clinical Study of a New Treatment Modality in Radiation Therapy
10:50-11:05	HPC-ORA-04	Pumipat Tongdom Kasetsart University	Differential equations learning from spatial-time series data by the fast iterative shrinkage thresholding algorithm
11:05-11:20	HPC-ORA-05e	Witcha Benjanirat Kasetsart University	Wavelet Gakerin Method for solving Korteweg-de Vries Equation with Neumann Boundary Conditions

POSTER SESSION

Thursday, 2nd August 2018
13:50-15:40, 3rd Floor, MHMK Building

Printed posters should be mounted beginning at 8:00 on Thursday 2nd Aug and MUST be removed by 18:00 on the same day. Posters are arranged according to research areas. There will be e-posters and printed posters.

Posters with an odd ID number should be presented from 13:55-14:45.
Posters with an even ID number should be presented from 14:45-15:35.

Computational Biology, Bioinformatics, Biochemistry and Biophysics Session

Code	Presenter	Title
BIO-POS-01	Nitchakan Darai Chulalongkorn university	*In silico* screening of chalcones against Epstein-Barr Nuclear Antigen 1 protein in Epstein-Barr virus.
BIO-POS-02	Jirayu Kammarabutr Chulalongkorn University	In Silico Studies on Potential Compounds against of Viral Hepatitis B Reverse Transcriptase
BIO-POS-03	Sasipha Seetin Kasetsart university	Binding investigation of pyrazine derivative against Glycogen synthase kinase-3 (GSK-3β) via in silico molecular dynamics simulations
BIO-POS-04	Nayana Bhat Chulalongkorn university	Molecular insights into substrate binding mechanism of Glycerophosphoethanolamine to Glycerophosphodiesterase.
BIO-POS-05	Kowit Hengphasatporn Chulalongkorn University	Homopharma-Based Identification Target of Phenolic Lipid Derivatives Against Dengue Virus Infected Cell
BIO-POS-06	Pitchayathida Mee-udorn Chulalongkorn University	Molecular Dynamics Study on Human Serine Hydroxymethyltransferase with Pyridoxal Phosphate Bound
BIO-POS-07	Peerapong Wongpituk Chulalongkorn University	Effect of Pyridoxal phosphate on Human Serine Hydroxymethyltransferaseby Molecular Dynamic Simulation
BIO-POS-08	Mattanun Sangkhawasi Chulalongkorn University	Effect of phenolic compounds as H5N1 influenza A neuraminidase inhibitors by molecular dynamic simulation
BIO-ORA-01e	Panupong Mahalapbutr Chulalongkorn University	Anticancer activity of mansonone G derivatives against human non-small cell lung cancer
BIO-ORA-02e	Bodee Nutho Chulalongkorn University	Reaction Mechanism of the Zika Virus NS2B/NS3 Serine Protease with Its Substrate: A QM/MM Study
BIO-ORA-03t	Wansiri Innok Thaksin University	The Potential of Interested Leading Alkaloid and Flavonoid Compounds in Thai Herbs against Achetylcholinesterase Inhibitory of Alzheimer's Disease
BIO-ORA-04e	Phakawat Chusuth Chulalongkorn University	The binding of cobratoxin from Naja kaouthia towards nicotinic acetylcholine receptor (nAChR)
BIO-ORA-05t	Tadsanee Awang Kasetsart University	Computational Studies of the Adsorption of Human Defensin 5 on Bacterial Membranes
BIO-ORA-06t	Channarong Khrutto Chulalongkorn University	Molecular Dynamics Simulations of M2 Channel in Phospholipid Bilayers with Different Thickness
BIO-ORA-07e	Kanyani Sangpheak Chulalongkorn university	In silico and in vitro studies of chalcones as potent anticancer agents with EGFR kinase
BIO-ORA-08e	Kanika Verma Chulalongkorn University	Exploring the Impact of R306C and F270V Mutations in β-Tubulin Structure and Function: A Computational Perspective
BIO-ORA-09e	Thapanar Suwanmajo Chiang Mai University	Tunable Signal Processing in Multi-site Phosphorylation Systems via Explicit Enzyme Activation

Computational Chemistry Session

Code	Presenter	Title
CHE-POS-01	Rathawat Daengngern King Mongkut's Institute of Technology Ladkrabang	Dynamics Simulation of Excited-State Intramolecular Proton Transfer Reactions of 2,5-bis(2'-benzoxazolyl) hydroquinone
CHE-POS-02	Tinnakorn Saelee Chiang Mai University	Theoretical investigation of Propane Dehydrogenation on Ni(111) surface
CHE-POS-03	Khanittha Kerdpol Chiang Mai University	Replica Exchange Molecular Dynamics Simulations of 2-Hydroxypropyl-β-Cyclodextrin
CHE-POS-04	Panisak Boonamnaj Chulalongkorn University	The pH-Dependent Shaping of Water-filled Crevice in the Hv1 Channel
CHE-POS-05	Rusrina Salaeh Chiang Mai University	Electronic and photophysical properties of derivatives of 2-phenylbenzothiazole and 2-(2′-hydroxyphenyl) benzothiazole: Effect of intramolecular hydrogen bonding
CHE-POS-06	Chattarika Sukpattanacharoen Chiang Mai University	Heteroatom effect on electronic and photophysical properties of 3-hydroxyquinolin-4(H)-one and its derivatives enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect
CHE-POS-07	Karan Bobuatong Rajamangala University of Technology Thanyaburi	Density functional theory insight towards the design of ionic liquids for CO2 capture
CHE-POS-08	Narissa Kanlayakan Chiang Mai University	Path Integral Molecular Dynamics Simulations for Muoniated Thioformaldehyde Radicals
CHE-POS-09	Panita Kongsune Thaksin University	Inhibitory of Influenza H1N1 Hemagglutinin with Flavonoid Compounds from Thai Herbs
CHE-POS-10	Bundet Boekfa Kasetsart University;	An ONIOM study on the 7-hydroxyl-4-methylcoumarin synthesis with H-Beta zeolite
CHE-POS-11	Jakkapan Sirijaraensre Kasetsart University	Effect of Impurities in MgCl2 Support for Polymerization of Ethylene with Heterogeneous Ziegler-Natta Catalyst: A DFT Study
CHE-POS-12	Pavee Pongsajanukul Chulalongkorn University	Computational calculation of CO2 adsorption in MIL-127(Fe) Metal Organic Framework
CHE-POS-13	Thanawit Kuamit Chulalongkorn university	ELECTRONIC PROPERTIES OF PYRENE ADSORBED ON GRAPHENE NANOFLAKES
CHE-POS-14	Chirawat Chitpakdee National nanotechnology center	Cooperation of Single Co Atom with Defect MoS2 as a High Efficient Catalyst for HDO Reaction: A DFT Study
CHE-POS-15	Warin Jetsadawisut, Chulalongkorn university	Molecular Dynamics Simulation of Nanodiscs using Coarse-Grained model
CHE-POS-16	Panichakorn Jaiyong Thammasat University	Computational Insight into Noncovalent Interaction of Solid Polymer Electrolytes on Graphene Surface for Fabrication of Supercapacitor Electrodes

Computational Chemistry Session

Code	Presenter	Title
CHE-POS-17	Anittha Prasertsab Kasetsart University	Lewis Acid Beta Zeolite Catalyzing the Catalytic Hydrogen Transfer of Furfural to Furfuryl alcohol: Insight from DFT Calculations
CHE-POS-18	Sarawoot Impeng National nanotechnology center	Theoretical investigation on gas sensing properties of a MnN4 moiety embedded graphene (MnN4-graphene)
CHE-POS-19	Fadjar Mulya Universitas Gadjah Mada	Design a Better Metalloporphyrin Semiconductor: A Theoretical Studies on the Effect of Substituents and Central Ions
CHE-POS-20	Sunan Kitjaruwankul Kasetsart University	3D-QSAR and molecular docking of xanthone derivatives as HIV-1 reverse transcriptase inhibitors
CHE-POS-21	Sarinya Hadsadee Ubon ratchathani university	D-π-A-π-A system with isoindigo for dye-sensitized Solar cells
CHE-POS-22	Teeranan Nongnual Burapha University	The Spatial Resolution in Fluorescent-Particle Tracking Affected by Motion Blur
CHE-POS-23	Noppakoon Kharmsri Chulalongkorn University	Dimer Interactions of H1V Proton Channel in Resting State by MolecularDynamics Simulations
CHE-POS-24	Suparada Kamchompoo Ubon Ratchathani University	Adsorption of hydrogen sulfide over metal exchanged zeolite clusters: A density functional theory study
CHE-ORA-01t	Nuttaporn Janprapa King Mongkut's University of Technology Thonburi	A theoretical study of fluorene based copolymers for solar cell applications
CHE-ORA-02t	Rattanawalee Rattanawan Ubon Ratchathani University	Molecular Engineering of D-A Featured Organic Indole Sensitizers for Improving Performance Efficiency of Dye-Sensitized Solar Cells
CHE-ORA-03e	Pipat Khongpracha Kasetsart University	Charge Carriers Distribution in Platinum Doped Graphitic Carbon Nitride Quantum Dot
CHE-ORA-04t	Yuwanda Injongkol Ubon Ratchathani University	The mechanism of carbon dioxide hydrogenation to formic acid on Pt-boron nitride nanosheets (Pt-BNNSs): A theoretical study
CHE-ORA-05t	Nuttapon Yodsin Ubon Ratchathani University	The theoretical study of catalytic CO2 hydrogenation to formic acid over a metal-decorated carbon nanocone
CHE-ORA-07t	Panyakorn Taweechat Chulalongkorn University	Molecular dynamics simulations of hyaluronic acid in water
CHE-ORA-09e	Wiparat Hotarat Chulalongkorn University	Delivery of Alpha-mangostin through biological membrane using cyclodextrins: A molecular dynamics simulation study
CHE-ORA-10e	Wasut Pornpatcharapong Chiang Mai University	Efficient Two-dimensional Ion Pairing Free Energy Surface Computation with Gaussian Process Regression
CHE-ORA-12e	Cangtao Yin Academia Sinica	The reaction between Criegee intermediates and sulfur dioxide: not really barrierless

Computational Physics, Fluid Dynamic and Solid Mechanics Session

Code	Presenter	Title
PHY-POS-01	Kunwithree Phramrung King Mongkut's University of Technology Thonburi	Meshless local Petrov-Galerkin (MLPG) method for HIV model
PHY-POS-02	Naravadee Nualsaard King Mongkut's University of Technology Thonburi	The Numerical Solution of Fractional Black-Scholes-Schrodinger Equation Using the MLPG Method
PHY-ORA-02e	Abdulmutta Thatribud Prince of Songkla University	Electronic and Optical Properties of Silver Chloride Photocatalyst by First Principles calculation
PHY-ORA-03t	Sorayot Chinkanjanarot National Metal and Materials Technology Center	Predicting Coefficient of Linear Thermal Expansion of Carbon Fiber/Graphene Nanoplatelet/EPON862 Hybrid Composites: Multiscale Modeling
PHY-ORA-04t	Somboon Otarawanna National Metal and Materials Technology Center (MTEC)	Matrix Tridiagonalization Methods for 3D Finite Element Analysis of Free Vibration
PHY-ORA-05e	Wanfeng Yu Mae fah luang university	Identify Transient Sources from GOTO Sky Survey Data with Clustering Method
PHY-ORA-06e	Vichayanun Wachirapusitanand Chulalongkorn University	Machine Learning system mimicking student's choice in Particle Data Analysis laboratory activity
PHY-ORA-07e	Maneerat Chotsawat Synchrotron Light Research Institute	First-principles study of defects in Bi and Al doped orthorhombic PbZrO3

High Performance Computing, Computer Science, Mathematic & Engineering Session

Code	Presenter	Title
HPC-ORA-01e	Piyakorn Phanklin Thammasat University	Loop prevention on Software Defined Network using Adaptive Virtual Tunnel Network
HPC-ORA-02e	Kanjanart Junnawat Thammasat University	Resilience flow management on Software-Defined Network using Directed graph for L2 Loop prevention
HPC-ORA-03e	Dussadee Somjaiwang King Mongkut's University	Existence and Approximation of Solutions of Coupled Fractional Order Hybrid Differential Equations
HPC-ORA-05e	Witcha Benjanirat Kasetsart University	Wavelet Gakerin Method for solving Korteweg-de Vries Equation with Neumann Boundary Conditions

PLENARY LECTURES

KEYNOTE SESSIONS
Plenary Lecture 1

Monte Carlo simulations of energetic particle transport in space, in Earth's atmosphere, and in a cosmic ray detector

David Ruffolo[1,C]

[1]*Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand*

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ABSTRACT

We present the results of Monte Carlo simulations to study cosmic rays, which are energetic particles from space. To better understand cosmic ray transport in space, we have performed numerical experiments on the random walk of magnetic field lines (e.g., [1]) and energetic particles (e.g., [2]) in turbulent magnetic fields and complex distribution patterns of energetic particles from solar storms in interplanetary space, providing some predictions for the upcoming Parker Solar Probe mission to approach close to the Sun [3]. To interpret data from ground-based cosmic ray detectors, we have used the FLUKA program to model atmospheric showers of secondary particles due to cosmic ray interactions in Earth's atmosphere, including estimates of atmospheric ionization and radiation doses of humans at aircraft altitude during a large solar storm [4]. We have also determined the sensitivity to secondary particles of the Princess Sirindhorn Neutron Monitor, a cosmic ray detector at Doi Inthanon, and can explain the absolute count rate to within 9% [5]. Furthermore, we also modeled the leader fraction (an indicator of the cosmic ray spectrum [6]) as measured by a neutron monitor on a ship during 2000-2006, and obtained very close agreement with the observed relative variation of the leader fraction [7].

Figure 1. Computing cluster at the Space Physics and Energetic Particles Laboratory, Department of Physics, Faculty of Science, Mahidol University

Keywords: Monte Carlo simulation, cosmic rays, energetic particle transport, radiation dosage.

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4. Mitthumsiri, W., Seripienlert, A., Tortermpun, U., et al., *J. Geophys. Res. Space Phys.,* 2017, **122,** 7946.
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7. Mangeard, P.-S., Ruffolo, D., Sáiz, A., et al., *J. Geophys. Res. Space Phys.,* 2016, **121,** 11620.

Prof. David Ruffolo received his B.S. in Physics and B.A. in Mathematics from the University of Cincinnati, USA in 1985, at age 17. He received his Ph.D. in Physics from the University of Chicago, USA in 1991, at age 23. He initiated space physics research in Thailand, where he has worked for the past 26 years. His awards include a 2014 Mahidol University Award for Research, a Senior Research Scholar Award from the Thailand Research Fund in 2016, and the 2017 Outstanding Scientist Award of Thailand.

KEYNOTE SESSIONS
Plenary Lecture 2

Future of High Performance Computing

Putchong Uthayopas
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ABSTRACT

Recent innovation in science and technology increasingly rely on the use of advance high performance computing system for the simulation, modelling and data analytics. The emerging trends in AI, Machine Learning and Data Intensive Science create the need for a much more powerful high performance computing system. Furthermore, power consumption, the change in application characteristics, and data intensive nature of modern applications have a strong effect on the design and structure of modern HPC system. This presentation intends to share the state of the art in HPC system design, the driving factors, and trends. The new challenges in HPC is identified and some approaches to solve the problem will be elaborated. Finally, the current trends regarding the design of exa-scale computing system will be presented.

Dr. Putchong Uthayopas is currently serving as Vice President for Information (CIO), Kasetsart University, Thailand. He works in High performance computing, Grid, and Cloud computing for more than 28 years. He publishes more than 160 papers in journals and conference proceedings. Dr. Putchong is the founding Director of Thai National Grid Center, Ministry of Information and Communication Technology (2006-2008). He also served as the President of Computational Science and Engineering Association (Thailand) during 2013-2015. Dr. Putchong is a recipient of the Distinguish Computer Engineer award in System Integration from the Engineering Institute of Thailand in 2012 for his contribution in Grid, HPC and Cluster computing work. He is a member of an advisory committee for Court of Justice (Thailand), NECTEC, Thailand Research Fund, NSTDA, NANOTEC, and many government agencies.

KEYNOTE SESSIONS
Plenary Lecture 3

Morphing structures and dynamics by a multigrain approach

R.B. Pandey
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ABSTRACT

A multicomponent system such as self-organizing flow of an immiscible fluid, bio-functionalization of nano-materials, and conformational response of proteins involves multi-scale dynamics and relaxations leading to well-defined morphing structures. Basic constitutive components may consist of particles (solvent), chains (polymer, peptide, and protein), platelets (clay, tethered membrane, graphene sheets) etc. with diverse shapes, sizes, and interactions. Relaxation of these constitutive units resulting from their stochastic movements and driving parameters such as temperature and field are critical in evolution of multi-scale structures. Although it is desirable, but often not feasible to incorporate all details from atomic scale in a large-scale computational modeling of many organizing systems and reach a desirable length scales needed to understand observables. Some degree of coarse-graining, therefore, becomes unavoidable in modeling of large-scale hierarchical assembly. Coarse-graining involves simplifying the complexity via approximations such as reducing the degrees of freedom and implementing efficient and effective computational methods. What and how to incorporate relevant details in coarse or fine-graining to explore a vast ensemble of phase space depends on specific issues.

Using multi-grained mechanism (e.g. simulated interactions, knowledge based data ensemble, and phenomenological interactions) we have examined organizing structures of a number of model systems over the years. Even with a simple particle constituents, one may be able to investigate self-organizing flow in a multi-component fluid and gain insight into linear and non-linear responses [1]. Bio-functionalization of a nano particle (Au, Pd, graphene) requires identifying appropriate peptides based on desirable characteristics, their binding propensity to specific target and stability; the functionalized nanoparticles can constitute a building block in designing smart materials with hierarchical structures for such application as sensing or drug delivery [2]. Investigating the scaffolding of peptides [3] could be useful in understanding such assembly as a templet for silica condensation by a marine microbe (diatom) in biomineralization [4].

Despite enormous interest in protein folding for decades, understanding of how a protein moves, relax, and conform to stable structures with prolific yet specific response remains an open question. Examples include membrane proteins such as unusual structural response of hHv1 and corA in their native and denatured phases [5, 6], self-organizing morphology of amyloid proteins such as lysozymes [7] etc. A number of local and global physical quantities such as the energy and density profiles, contact and mobility maps, mean square displacements, radius of gyration, and structure factor are analyzed to understand multi-scale characteristics. Some of our findings from simplified coarse-grained models augmented by fine-grained data will be presented as time permits.

Keywords: Coarse-grained models, multi-component systems, bio-nano materials, protein folding.

Acknowledgement: RBP acknowledges generous support from the Chulalongkorn University where some of the recent work is performed in our on-going collaboration with the research group of Prof. Pornthep Sompornpisut. Warm hospitality of the Chemistry Department at the Chulalongkorn University is gratefully acknowledged.

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Prof. Pandey received his Ph.D. from IIT Roorkee in 1981 and worked at the North Carolina State University (1981-1982) as a visiting assistant professor before his postdoctoral work at Cologne University (1983), University of Cambridge (1984), University of Georgia (1984). He became assistant professor at the Jackson State University in 1985 and moved to University of Southern Mississippi (in 1988) where he is professor of physics for about 30 years. His research spans over a wide range of application of statistical physics (transport and flow of fluid in porous media, polymer, interface and roughness, nano-bio-composites, protein). He has over 150 papers in refereed journals. He was awarded Alexander von Humboldt fellowship early in his career and recently became a fellow of the American Physical Society. He is an academic editor of AIP Advances (American Institute of Physics) and has served in several national and international scholarly committees (research funding, program review, promotion etc.) and collaborated with many research groups around the world.

Workshop on Ab Initio Simulation of Reaction Rates and Vibrational Spectra

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ABSTRACT

Due to advances in quantum chemistry Ab Initio methods, we can theoretically model reaction rates and provide predictions for gas phase reactions. In this workshop, we will review basic concepts such as Born–Oppenheimer approximation, as well as review the basic concepts used in ab initio packages. Furthermore, we introduce important aspects in the calculation of the vibrational and rotational partition function to accurately simulate thermal reaction rates. The accuracy of the vibrational calculation will be shown through the comparison with experimental vibrational spectra. I hope to provide some background on rate simulations as well as some tricks that are being used.

Kaito Takahashi is a Japanese theoretical chemist working as an associate research fellow at the Institute of Atomic and Molecular Sciences, Academia Sinica (IAMS, AS) Taiwan. In 2005, he obtained his Ph.D. from Keio University under the tutelage of Prof. Satoshi Yabushita. After four years of postdoctoral fellow research under Prof. Rex. T. Skojde, he started his lab at IAMS in 2009. His scientific interest for the past few years has been to theoretically understand properties that control reactions and to simulate vibrational, photodetachment, and X-ray absorption spectra. In 2017, he received the Academia Sinica Career Development Award for his theoretical studies on Criegee intermediates.

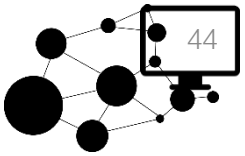
ABSTRACT

I) Computational Biology, Bioinformatics, Biochemistry and Biophysics: **BIO**

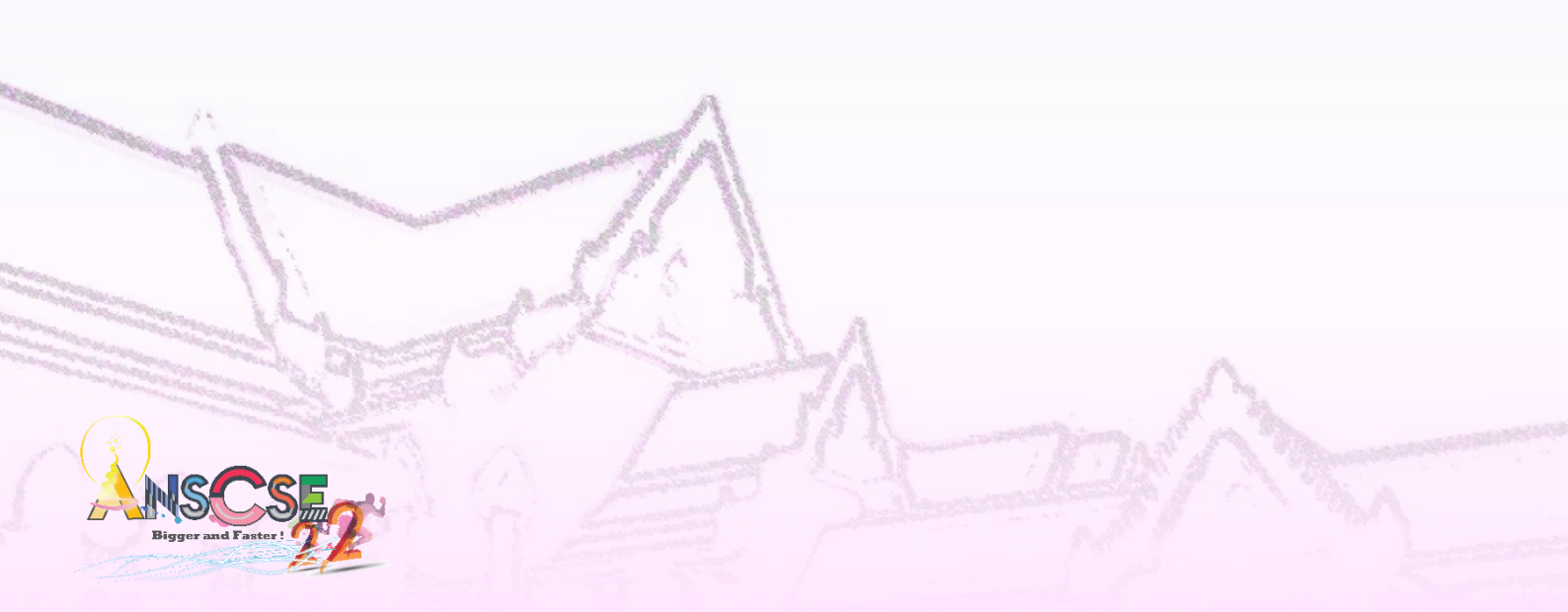
II) Computational Chemistry: **CHE**

III) Computational Physics, Computational Fluid Dynamics and Solid Mechanics: **PHY**

IV) High Performance Computing, Computer Science, Mathematics and Engineering: **HPC**



I) Computational Biology, Bioinformatics, Biochemistry and Biophysics



Data-driven Parallel Cascade Selection Molecular Dynamics

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ABSTRACT

Recently, the small angle scattering method (SAXS) has attracted much attention in the field of biomolecular structural analyses, because it does not require crystals for the sample and can exceed the upper limit of the molecular weight (though not limitless) in solution. Cryo-electron microscopy (EM) is also increasingly becoming a mainstream technology for studying not only proteins but also larger biomolecular systems such as viruses and cells. In spite of their powerfulness, these methods lack detailed atomic resolution of the structures. Therefore, it is expected that the obtained structures will be refined with computer modeling. For the structural refinements based on the SAXS data or EM maps, several computational methods for constructing high-resolution structures have been developed. However, in order to understand the protein dynamics related to the protein function, one wants to know the structural transition among obtained stable structures.

For this purpose, we have proposed a computational method to promote conformational transitions of proteins, which is referred as Parallel cascade selection molecular dynamics (PaCS-MD) [1]. PaCS-MD accelerates to find transition pathways between a given reactant and a product by repeating the following two steps: (1) selections of initial structures relevant to transitions and (2) their conformational resampling (see a review for detail [2]). When selecting the initial structures, several measures are utilized for identifying their potentials to make transition. In the present lecture, low-resolution structural data obtained from SAXS and cryo-EM are adopted as the measures in PaCS-MD to promote the conformational transitions of proteins, which are defined as SAXS-/EM-driven targeted PaCS-MD. By selecting essential structures that have high correlations with the low-resolution structural data, the SAXS-/EM-driven targeted PaCS-MD identifies a set of transition pathways between the reactant and the product. As a demonstration, the present method successfully predicted the open-closed transition pathway of the lysine-, arginine-, ornithine-binding protein with a ns-order simulation time, indicating that the data-driven PaCS-MD simulation might work well to promote conformational transitions of proteins efficiently.

Keywords: Biophysics, Molecular Dynamics Simulation, Data Assimilation.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-02

Simulational studies of Aβ amyloid fibrils by molecular dynamics method

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ABSTRACT

Amyloids are insoluble and misfolded fibrous protein aggregates and associated with more than 40 serious human diseases. For example, amyloid-β fibrils (Aβ) are known to be associated with the Alzheimer's disease. We performed molecular dynamics (MD) simulations of Aβ fibrils in explicit water. We discovered that molecular structure is different between two ends: The two β-sheets β1 and β2 are close to each other. On the other hand, at the odd end the Aβ peptide fluctuates more and takes an open form, too [1]. Our theoretical prediction was proved by experiment after our MD simulations.

We also performed nonequilibrium molecular dynamics simulations of an Aβ fibril in explicit water under supersonic wave to mimic some experimental reports that cavitation disrupts amyloid fibrils [2]. We found that when the pressure was decreased to a negative value, a bubble formation was observed. When the pressure was increased to a positive value, water molecules attacked the hydrophilic residues, the bubble collapsed, and the fibril was disrupted.

Keywords: Molecular Dynamics, Amyloid Fibril.

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Hisashi Okumura was born in 1975 and got his Ph.D. degree from Faculty of Science and Engineering, Keio University. He moved to University of Tokyo as a postdoctoral fellow of the Japan Society for the Promotion of Science for Young Scientists. He then moved to Institute for Molecular Science as a research associate. After he worked at Rutgers University in USA, got his present position of associate professor at Institute for Molecular Science.

Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-03

Molecular dynamics simulations of a full-length amyloid-b peptide at a hydrophobic/hydrophilic interface

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ABSTRACT

The amyloid-b peptide (Ab) is composed of 39–43 amino-acid residues. Ab tends to form amyloid fibrils, which are associated with the Alzheimer's disease. It was reported that formation of amyloids is accelerated at a hydrophobic/hydrophilic interface such as an air/water surface or an interface between sugar-head groups and hydrocarbon chains of glycolipids [1–3]. It is necessary to clarify the amyloid formation process at the interface in order to find a remedy for Alzheimer's disease. To investigate amyloid formation process at the hydrophobic/hydrophilic interface, we performed molecular dynamics (MD) simulations for a full-length Ab molecule, Ab40, in the presence of the solution surface. For comparison, MD simulations of Ab in bulk water were also performed.

Figure shows the average distances of the C_a atoms from the interface. As shown in the figure, residues in the b1 region (residues 10–22) and the b2 region (residues 30–40) existed in the vicinity of the solution surface. Furthermore, these residues tended to form helix structures as reported in experiments [3]. In my presentation, other simulation results will be shown, and solution surface effects on the amyloid formation process will be discussed.

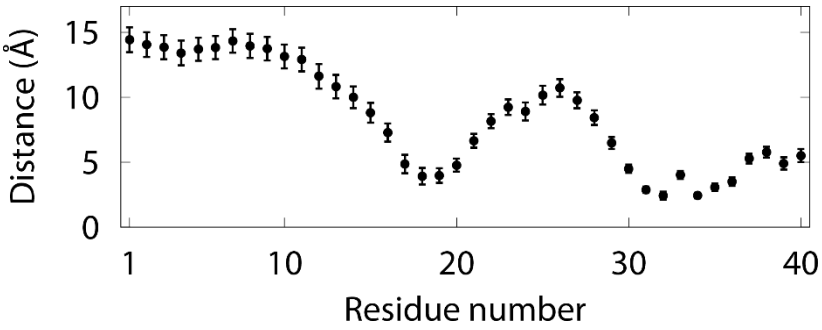

Figure Average distances of the C_a atoms from the solution surface.

Keywords: Amyloid-beta peptides, Molecular dynamics simulation.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-04

Quantum Calculations on the Voltage Sensing Domain of a Voltage Gated Ion Channel

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ABSTRACT

A key question in physiology that remains not clearly resolved is the gating (opening and closing) mechanism of the ion channels that produce the nerve impulse and determine many other biological functions. Channel opening is preceded by a small capacitative current (gating current); we propose that the gating current consists of the transfer of protons through the voltage sensing domain (VSD) of the channel; the more generally accepted model has a positively charged helix moving as a whole, rather than protons. We present evidence based on quantum calculations, primarily done on a 976 atom cluster cut from the VSD of a K_v1.2 voltage gated potassium channel. The first step was optimization, at HF/6-31G* level, of the structure of the cluster, starting from the X-ray experimental structure. The energy and other properties of the optimized structures were then calculated at B3LYP/6-31G** level, with NBO used to determine the bond orders and atomic charges[1]. Two particular hydrogen bonds made a major contribution to the transition from closed to open channel. The system was calculated at several transmembrane fields, which corresponded to voltages from -70 mV (closed channel) to +70 mV (≥0 mV produces an open channel). A Y→F mutant, removing –OH while keeping the volume constant, was also tested. This prevents the transfer of a proton among certain amino acid residues internal to the cluster. The mutant has been tested experimentally (we thank Professor F. Bezanilla and Dr. C. Bassetto for permission to quote their data), and the prediction was at least qualitatively correct; there was an approximately 1.7-fold decrease in slope of the gating current-voltage curve. The calculations also found nearly quantitative agreement between the extent of depolarization required to transfer the proton and the depolarization required to open the channel, supporting the proton transfer to gating connection. The QM exchange and correlation energies were greater than kT, and their differences in the different proton positions were also greater than kT; a classical calculation would give a very different transfer depolarization. We will briefly comment on the comparison of QM cluster calculations with QM/MM and other possibilities; as we did not actually carry out such calculations, only qualitative comparisons can be discussed. It appears that the single cluster is most likely to be reliable, especially for transitions not near the boundary of the cluster. Otherwise it would be necessary to terminate the cluster in a smaller region, which requires adding hydrogen to close the truncated bonds. The difficulties that accompany the outer (classical) portion, and its boundary with the inner section, appear to make the system more inaccurate than the simple cluster, even though it would include many more atoms. The errors in hydrogen bonds alone would alter the hydrogen transfer that is central to the calculation. This type of calculation will benefit more than any other from increases in computer capability.

Keywords: Quantum calculations on a protein; computations on voltage gating

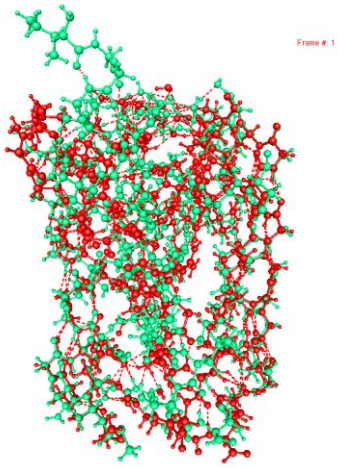

Figure The optimized VSD structure (red) shows no downward motion of a protein helix compared to X-ray structure (green), when a polarizing field is applied, equivalent to the potential across the membrane with the channel closed.

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My undergraduate degree is from Cornell, PhD Yale, postdoc Caltech (with Wilse Robinson). After teaching for 2 years (1964-66) at Middle East Technical University(Ankara), I have spent the last 52 years on the chemistry faculty at the City College of the City University of New York. Over the last 30 years, I have worked on computations of the gating mechanism in voltage gated ion channels, proposing that the gating current is the motion of protons. Quantum calculations appear to be required for credible results.

Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-05

Theoretical study of biological processes employing statistical mechanics of molecular liquids

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ABSTRACT

Life phenomena are a series and a network of chemical reactions, which are regulated by genetic information inherited from generation to generation. The genetic information itself is generated and transmitted by a series of chemical processes. In each of those reactions, some characteristic process takes place, which distinguishes biochemical reactions from ordinary chemical reactions in solutions. Such a process is referred to as molecular recognition (MR). MR is an extremely selective and specific process in the atomic level, and that selectivity as well as specificity plays a key role for living systems to maintain their life. MR is a molecular process determined by specific interactions between atoms in host and guest molecules. On the other hand, the process is a thermodynamic process as well, with which the chemical potential or the Gibbs energy of guest molecules in the recognition site and in the bulk solution are concerned.

A theoretical approach to MR has been launched based on a three-dimensional reference interaction site model (3D-RISM) method.[1] By solving 3D-RISM equations, we can obtain the solvation structure around a solute. The theory has been successfully applied to such MR problems as probing ligand molecules caged in protein, ion binding by protein, and the ion conduction through the channels.

The electronic structural changes of ligand and receptor molecules are another serious concern in MR processes. Recently, we proposed an efficient implementation of 3D-RISM to the electronic-structure theory of macromolecules such as fragment molecular orbital (FMO) and quantum mechanics/molecular mechanics (QM/MM) methods.[2,3] These methods are referred to as FMO/3D-RISM and QM/MM/RISM, respectively. They allow us to treat an electronic structure of macromolecules, such as protein, as well as a solvent distribution around the solute macromolecules. In the presentation, we review our recent studies on the molecular recognition by protein based on 3D-RISM and its extensions.

Keywords: 3D-RISM, QM/MM, FMO

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Norio Yoshida was born in Gunma, Japan, in 1973. He received his M. S. degree from Kyoto University in 1999, and earned his Ph.D. degree in theoretical chemistry from Kyoto University in 2003. At present, he is Associate Professor at Department of Chemistry, Graduate School of Sciences, Kyushu University. His research interest includes theory of solvent effects on electronic structure of molecule and molecular thermodynamics in solution.

Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-06

Structure and conducting mechanism characterization of DNA template guided nickel ion chain

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ABSTRACT

DNA is a self-assembled dimeric molecule which storage the genetic information of cell. A two micro-meter long DNA molecule was used as the template to aligned nickel ions within its structure. Extended X-ray absorption fine structure analysis and structural optimization indicated that a Ni-DNA complex chain (Ni-DNA) was fabricated. Molecular orbital analysis of Ni-G-C base pair indicated both nickel ion and base-pair participate charge transport within Ni-DNA. Namely, the charge transport through the pi-pi stacking corridor or Ni-DNA. Furthermore, the redox state of each nickel ion in Ni-DNA can be programmed by applying different polarities and writing time of bias voltages. The multi-state information can be written, read, and erased on this Ni-DNA memristive and memcapacitive system. Thus, this Ni-DNA conducting nanowire can be used as memelemet for memory computing (mem-computing).

Keywords: Ni-DNA, strcutral optimization, memristor, memcapacitor, memcomputing.

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Professor Chia-Ching Chang is a Biological Physicist. Professor Chang is the Chairman of Dept Biol. Sci & Tech., NCTU. At the same time Prof. Chang was co-appointed as Research Fellow by Institute of Physics, Academia Sinica, Taiwan. The research topics of Dr. Chang include: Soft condense matter and Biological physics; Functional biomaterials synthesis and characterization, Bio-nanotechnology and Biophotonics.

Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-07

Biocompatible MOFs for Drug Delivery: Computational Studies.

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ABSTRACT

A group of Metal organic frameworks (MOFs) like Material of Institut Lavoisier (MIL) family is investigated as a potential drug delivery system due to its porosity and biodegradable properties. In this study, some MIL-framework such as MIL-58 and MIL-127 are used as host for drugs encapsulation. The adsorption isotherm, binding energies, diffusions and some structural properties are obtained by quantum calculations and computer simulations.

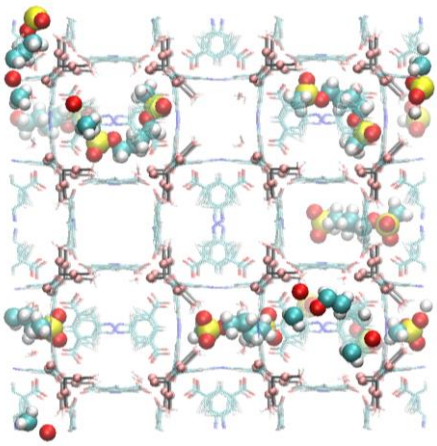

Figure 1. Busulfan molecules inside MIL-127 which is obtained by MD simulations.

Keywords: MOFs, MILs, Flexible MOFs model, drug delivery.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-08

Catalytic Roles of Histidine and Arginine in Pyruvate Class II Aldolase

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ABSTRACT

The retro-aldol reaction catalyzed by pyruvate class II aldolase is investigated with QM/MM metadynamics. The pyruvate class II aldolase transforms the substrate of 4-hydroxy-2-ketoacid into pyruvate and aldehyde through the aldol cleavage. Simulations are focused on the structures of 4B5V, 4B5U and 4B5W. The hydroxyl group of the substrate is deprotonated by His45 with the aid of the metal-bound water, while the metal-bound hydroxide proposed in the literature[1] is observed as a transient species. The deprotonation appears to enhance substrate binding between the deprotonated substrate and the active site. The reactive alkoxide is further stabilized by the salt bridge formed by Arg70−Asp42, facilitating the following aldol cleavage. Computations show that the C−C bond cleavage is the rate-determining step, and the calculated barrier[2] (Figure 1) of 13.7 kcal/mol agrees reasonably with experimental data.[3]

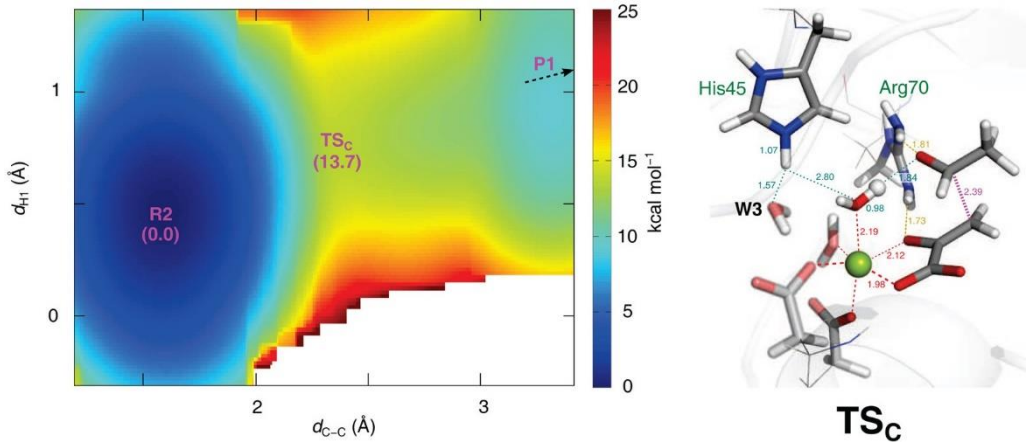

Figure 1. Free energy landscape for the step of C−C bond cleavage.

Keywords: Retro-Aldol Reaction, Pyruvate Class II Aldolase, QM/MM Metadynamics.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-INV-09

Toward Next-Generation Neoantigen Prediction with Deep Learning

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ABSTRACT

Immunotherapy is a promising cancer treatment that activates the patient's own immune system to recognize and destroy his/her tumor cells 1. This technique relies on the premise that, with proper stimulus, mutated proteins in a cancer cell would be detected by the host's immune system as "foreign" in the same way that viral proteins in infected cells do. One such approach involves purposely injecting vaccine that consists of peptides with the same mutations as in the patient's own tumor 2. Due to technical difficulty and the sheer number of mutations in each tumor, the ability to predict whether a mutated peptide would be bound to the human leukocyte antigen (HLA) complex and ultimately recognized by T-cell is absolutely essential. In the first phase of this work, we trained a deep neural network model for predicting peptide-HLA binding that not only outperforms current leading neoantigen predictors but also is able to handle new HLA types. Nonetheless, because the pathway for presenting mutated peptides on cancer cell's surface involves much more than just binding to the HLA proteins themselves, high HLA binding affinity does not necessarily translate to being effective neoantigen. A potential remedy is to train future models using primarily HLA peptidomes 3,4 where detected peptides must have gone through an antigen presentation pathway for the most part. In this aspect, we are also applying deep learning 5 to improve the quality and coverage mass spectrometry-based peptide identification to refine HLA peptidome datasets.

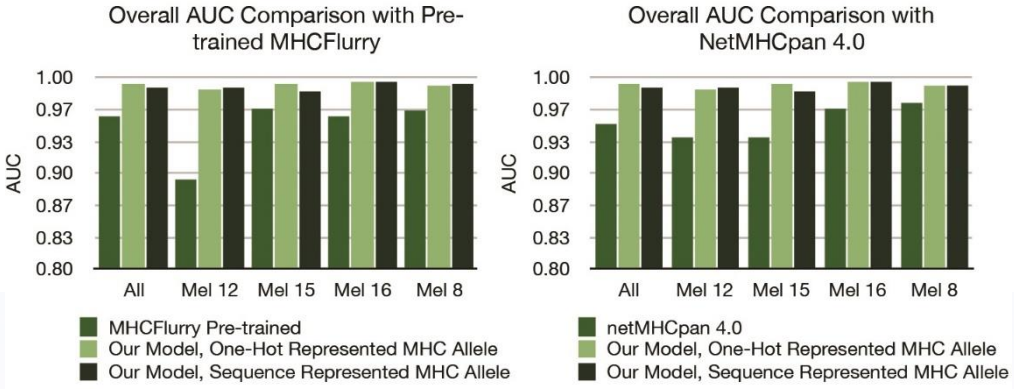

Figure Performance comparison between our deep learning model and current leading neoantigen predictors on a class I HLA peptidome dataset [4]

Keywords: Neoantigen Prediction, Deep Learning, Computational Biology.

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Sira Sriswasdi is currently a lecturer at Chulalongkorn University, Thailand, where his Computational Molecular Biology research group collaborates with experimental laboratories to answer biological and medical research questions using machine learning and mathematical modeling techniques. His current projects aim at improving mass spectrometry-based peptide identification and elucidating the evolutionary processes of fungal and viral genomes.

The relationship between protein function and local structural conservation

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ABSTRACT

The protein-molecule interaction plays an essential role in almost all cell function. To identify functional structural motifs from the protein-molecule interaction becomes extremely important in recent years due to the progress of the structural genomics projects. In practice, the functional structural motifs have highly constraints in structural and physical properties. For example, the Asp-His-Ser catalytic triads are easy to detect because of their conserved residues and stringently constrained geometry. The helix-turn-helix motif is a common recognition structural motif used by transcription regulators. The bba-metal binding motif plays a crucial role in non-specific DNA interactions and cleavage in host defense and apoptosis. The treble clef motif is a zinc-binding motif adaptable to diverse functions such as the binding of nucleic acid and hydrolysis of phosphodiester bonds. According to these properties, the ability to identify functional structural motifs is important in predicting protein function and in providing a complementary tool to the fold alignment method.

Up to present, there are more than 130,000 structures in Protein Data Bank (PDB) and several computational methods are designed for structure alignment. However, most structure alignment methods are failed to return results for local structural motifs which are composed of relatively short and discontinuous fragments. Hence, we have developed a novel method to detect the structural motifs or protein-molecule interaction sites from protein structure[1-4]. This method is called the fragment transformation method which is a local structural alignment algorithm combining both structural and sequence information to identify the local structure motifs. It should be noted that the short and discontinuous fragments of protein can also be processed by our approach. We have already applied our method to detecting several structural motifs and ligand binding sites, such as the bba-metal motif[1], the treble clef finger motif1, metal ion-binding sites[2, 3], Flavin and Nicotinamide Adenine Dinucleotide (FAD/NAD) binding sites[4]. The results were encouraging, indicating that the functional structural motifs can be effectively identified by the fragment transformation method. Moreover, our method provided a useful, effective means for automatic function annotation of structural genomics research through detecting structural motifs associated with particular functions.

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Anticancer activity of mansonone G derivatives against human non-small cell lung cancer

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ABSTRACT

Lung cancer is the first leading cause of mortality worldwide. More than 85% of all diagnosed cases are currently classified as non-small-cell lung cancer (NSCLC) [1]. Platinum-based doublet chemotherapy (i.e., cisplatin) and the 1st generation tyrosine kinase inhibitors (i.e., erlotinib) have been used as the first-line treatment for NSCLC patients carrying wild-type and L858R-mutated epidermal growth factor receptor (EGFR), respectively. However, the multidrug resistance often develops during treatment, including (i) the over-expression of copper transporter and (ii) the secondary mutation T790M of EGFR can eventually lead to treatment failures [2]. Accordingly, searching for a novel compound that can potentially inhibit the NSCLC proliferation is critically needed. In the present study, mansonone G (MG) and its derivatives were screened toward A549 human NSCLC cell line, which expresses wild-type EGFR, using MTT assay. In vitro screening results reveal that among 10 MG derivatives, MG3 exhibits the great cytotoxicity against A549 cell line and it is relatively safe for normal cells. The western blot analysis reveals that MG3 inhibits signal transducer and activator of transcription (STAT) and phosphatidylinositol 3-kinase (PI3K)/Akt signaling pathways, leading to cell apoptosis. Moreover, the binding affinity of MG3 in complex with STAT, Akt, and Erk proteins was investigated in comparison with known inhibitors using MD simulations and MM/PB(GB)SA calculations.

Keywords: Non-small cell lung cancer, Cisplatin, Quinone

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Reaction Mechanism of the Zika Virus NS2B/NS3 Serine Protease with Its Substrate: A QM/MM Study

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ABSTRACT

Zika virus (ZIKV), a mosquito-borne flavivirus, was originally isolated from sentinel rhesus monkey in the Zika Forest of Uganda in 1947. The virus is transmitted to humans by *Aedes* species mosquitoes. The recent reports have revealed that this virus is now associated with serious pathological disorders including microcephaly in newborns and Guillain-Barré syndrome in adults. Unfortunately, there are no currently available vaccines or therapeutic drugs for preventing or controlling ZIKV infection. One of the attractive drug-targets for ZIKV treatment is the nonstructural (NS)2B/NS3 serine protease that processes viral polyprotein during infection.[1] Here we have used a hybrid Quantum Mechanics and Molecular Mechanics (QM/MM) umbrella sampling simulation at the PM6/Amber ff14SB level of theory to investigate the acylation step of the reaction catalyzed by the enzyme. The QM/MM umbrella sampling simulations indicate that proton transfer from Ser135 to His51 and nucleophilic attack on the substrate by Ser135 occur in a concerted reaction mechanism (Figure 1). The rate-limiting step is marked as the tetrahedral intermediate formation with an energy barrier of ~10.0 kcal/mol lower than the experimentally determined activation energy (16.2 kcal/mol)[2]. Nevertheless, the ability of the QM/MM presented here could be informative and useful for further designing of NS2B/NS3 inhibitors based on transition state analogues.

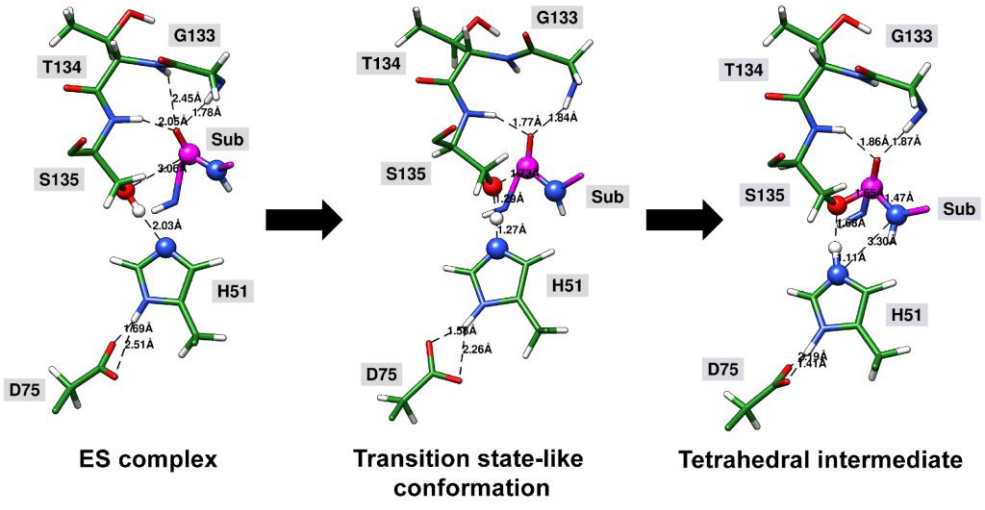

Figure 1. Structures of the three states in the reaction. Important distances are indicated in black dash lines.

Keywords: Enzyme catalysis, NS2B/NS3 serine protease, QM/MM reaction mechanism, Zika virus.

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The Potential of Interested Leading Alkaloid and Flavonoid Compounds in Thai Herbs against Achetylcholinesterase Inhibitory of Alzheimer's Disease

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ABSTRACT

Alzheimer's disease (AD) is the most common dementias. Most of patients are found in the elderly population, older than 65 years old. One of the mechanisms of AD involves the reduction in acetylcholine (ACh), a neurotransmitter of the cholinergic system, which involved in memory formation. Acetylcholinesterase (AChE) is a serine hydrolase enzyme family that plays a key role in the ACh hydrolysis and leads to the decrease of ACh. AChE plays an important role in AD. Currently, four drugs (tacrine, dopenzial, galantamine, and rivastigmine) that act as AChE inhibitors (AChEI) are used for the treatment of AD. However, these drugs are known to induce several side effects such as gastrointestinal disturbances, and they have low bioavail-ability. Hence, it is urgent to develop better inhibitors of AChE from natural sources to treat AD without any side effects. Therefore, this study aims to identify alternative drug molecules from natural products for treating AD, by evaluating the potential of alkaloid and flavonoid compounds for AChEI by using molecular docking simulation studies were performed to predict binding energies and identify the interacting residues of the selected alkaloid and flavonoid compounds with AChE. In addition, there is also the *In vitro* cholinesterase assays, by evaluate the anti-AD activities of selected alkaloid and flavonoid compounds according to inhibitory of AChE was performed. Molecular docking simulation studies and *In vitro* cholinesterase assays demonstrated that alkaloid compounds have significant inhibitory the potential against AChE. Moreover, the result of molecular docking studies revealed potential AChE inhibitory activity of alkaloid, especially Mitragynine oxindole B, which exhibited good binding affinities toward AchE, with docking scores of –11.52 kcal/mol.

Keywords: Alzheimer' disease, Alkaloids, Flavonoids, Molecular Docking, Acetylcholinesterase Inhibitors.

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The binding of cobratoxin from Naja kaouthia towards nicotinic acetylcholine receptor (nAChR)

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ABSTRACT

Thai cobra or *Naja kaouthia* is one of Thailand's most deadly snake. It lives across Thailand and a single bite can cause death. Cobra venom attacks the neurotransmission at the postsynaptic cell, i.e., postsynaptic neurotoxin. One of the main neurotoxins is cobratoxin or long α neurotoxin. It consists of 71 amino acids with five cross-linked disulfide bonds. It showed the high affinity in the binding with chicken α7 nicotinic acetylcholine receptor (nAChR) with Kd in nM range. From number of previous studies in both crystallization and site-directed mutagenesis, this toxin was found to bind at extracellular domain (ECD) of nAChR. Since no crystal structure of cobratoxin in complex with human α7 nAChR is currently available, understanding how cobratoxin binds towards human α7 nACh would be beneficial to develop the monoclonal antibody. Herein, we have performed all-atom molecular dynamics (MD) simulations on nAChR ECD homopentamer with a cobratoxin bound. From over 100 ns, cobratoxin interacted strongly with nAChR at C-loop and β2 strand mainly through its loop II. A key binding residues (Y210 of nAChR and D27, A28, F29, R33, K35, R36, F65 of cobratoxin) were similar to those experimentally determined in chicken α7 nAChR and acetylcholine binding protein (AChBP) of *Lymnaea stagnalis*. However, the F-loop of cobratoxin was not the binding site as proposed by previous studies.

Keywords: nAChR, cobratoxin, long alpha neurotoxin

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-ORA-05t

COMPUTATIONAL STUDIES OF THE ADSORPTION OF HUMAN DEFENSIN 5 ON BACTERIAL MEMBRANES

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ABSTRACT

Human α-defensin 5 (HD5) is one of the important anti-microbial peptides (AMPs) used against a broad-spectrum of pathogens in human, especially Gram-negative bacteria. HD5 kills by disrupting and making a pore in the bacterial membrane. A presence of lipopolysaccharide (LPS), located on a membrane surface, is found to have an impact on HD5's activity where the binding mechanism remains unclear. In this work, we therefore employed Molecular Dynamic (MD) simulations to investigate the binding mechanisms of HD5 on both LPS and bare lipid membranes. The activities of both stable HD5 forms (dimer and tetramer) were investigated in comparison. We observe that the chemical properties of membrane surface influence the binding affinity of HD5. Both dimeric and tetrameric HD5 can penetrate deeply into a phosphate layer in a lipid membrane, whereas HD5 only sits on a LPS membrane. Furthermore, residues in the active region (A1, T2, R6, R13, R32) appear to play a key role in membrane adsorption in all cases. Our results also show that the dimer is more desirable on a membrane. Moreover, both dimeric and tetrameric HD5 can significantly disrupt the LPS layer, whilst no serious distortion of lipid membrane is obtained. This emphasizes the importance of LPS on HD5 activity. This information is not only useful for better understanding our immune system, but also serve as a guidance for further design and development of antimicrobial drugs.

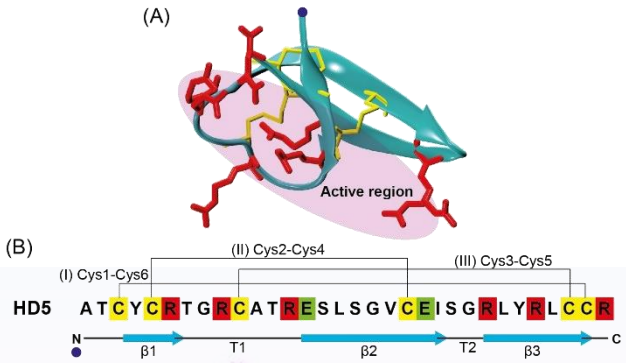

Figure 1 (A) Cartoon view of monomeric HD5. The disulfide bridges and key arginine residues are in yellow and red. The arginine-rich region ("the active region") is displayed in pink circle. (B) amino acid sequences of HD5. Conserved cysteine residues are shown in yellow, positively-charged residues are printed in red, and anionic residues in green. Key disulfide bonds are also shown.

Keywords: Antimicrobial peptides, Human α-defensin 5, Lipopolysaccharide, Molecular dynamics simulations, Host-defense peptide.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-ORA-06t

MOLECULAR DYNAMICS SIMULATIONS OF M2 CHANNEL IN PHOSPHOLIPID BILAYERS WITH DIFFERENT THICKNESS

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ABSTRACT

M2 channel is an integral membrane protein ion channel which has an important role in transferring proton across the membrane. M2 channel is an important protein in replication of influenza A virus. Structure of M2 channel is a tetramer. Each monomer consists of 97 residues. The residues 24-46 form an alpha helix embedded in the membrane. It is called transmembrane segment. Three-dimension structure of the M2 channel from X-rays crystallography technique and nuclear magnetic resonance technique (NMR) provides useful information that could lead to an understanding of molecular mechanism underlying the proton transport of M2 channel. The information can be useful for drug design and discovery.

Structural information from electron spin resonance spectroscopy technique (ESR) show that the M2 channel undergoes conformational changes when it has been constituted in different types of phosphatidylcholine lipids. However, details at the molecular level from ESR data is limited. In this study, we performed using molecular dynamic simulation (MD) of the viral M2 channel in different phospholipid bilayer to examine changes in transmembrane rearrangement of M2. We found that the thickness of phosphatidylcholine has induced changes in the conformation of M2 channel in a way that is contradict to experimental report.

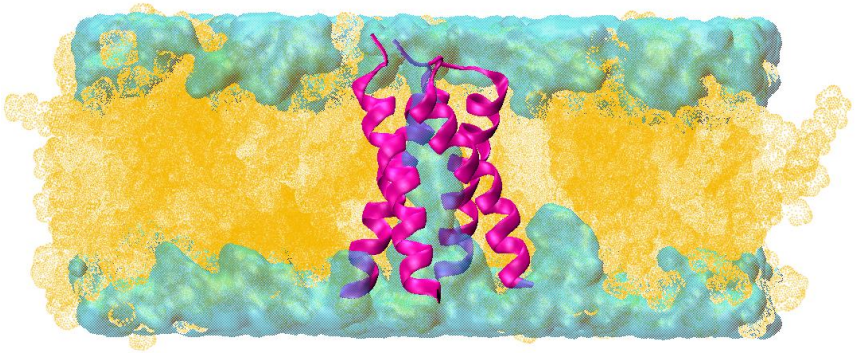

Figure 1. Conformation of M2 protein channel in MD simulation

Keywords: M2 protein channel, Influenza A virus, molecular dynamics simulation.

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In silico and *in vitro* studies of chalcones as potent anticancer agents with EGFR kinase

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ABSTRACT

The epidermal growth factor receptor (EGFR, Fig. 1) is one of molecular targets for anticancer therapy. It is overexpressed in many human cancer cells including non-small cell lung, breast, head and neck, bladder, ovarian carcinoma and especially skin (A431) cancer cell lines [1]. Chalcone (1,3-diphenyl-2-propen-1-one) is a phenolic compound abundant in edible plant and is considered to be a precursor of flavonoids. The pharmaceutical activities of chalcones such as anti-proliferative, antioxidant, anti-inflammatory and anti-cancer activities have been reported [2]. Some chalcone derivatives were found to inhibit EGFR. In this study, cell-based and enzyme assays were used for screening potent compounds from the 47 synthesized chalcones. As a result, the chalcone **2a** inhibits A431 cancer cells and EGFR activity with IC50 values in micromolar range. It shows less cytotoxicity toward the human embryonic fibroblast than commercial drug, erlotinib. In addition, the computational simulations were applied to investigate how this anticancer drug candidate inhibiting the EGFR kinase.

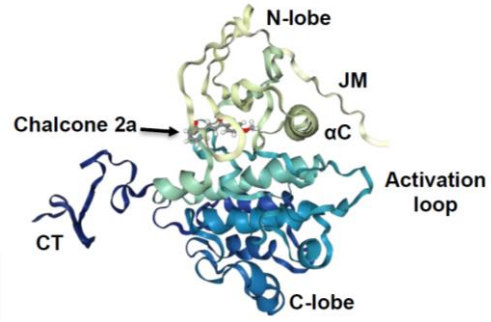

Figure 1. Docked structure of chalcone **2a** in the binding site of EGFR kinase domain

Keywords: Chalcones, Anticancer activity, EGFR kinase assay, MTT assay, Computational simulations

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Exploring the Impact of R306C and F270V Mutations in β-Tubulin Structure and Function: A Computational Perspective

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ABSTRACT

Paclitaxel is the most effective chemotherapeutic agent used for the treatment of a broad spectrum of solid tumors. However, observed paclitaxel resistance in clinical trials presents one of the major obstacles for cancer chemotherapy. Most importantly, resistance due to β-tubulin mutations (R306C, F270V) has been intensely debated in recent years. Despite all efforts, mechanism of resistance is still not well understood. In this study, computational techniques were employed to uncover the effect of R306C and F270V mutations in the β-tubulin structure and its function. The tools such as I-Mutant and CUPSAT were employed to address the consequence of R306C and F270V mutations in the structural stability of β-tubulin. Further, molecular docking and molecular dynamics study was employed to understand the functional impact of β-tubulin mutations. Our results suggest that the R306C and F270V mutation causes a significant reduction in the binding affinity between β-tubulin and paclitaxel. Further, docked complex analysis indicates that destruction of conservative hydrogen bond maintained by the residues Arg282 and Gly360 should be responsible for the large conformation changes of the binding pocket in R306C and F270V mutants. Finally, molecular dynamics simulations study confirms the stable binding of paclitaxel with native type β-tubulin structure rather than mutant (R306C, F270V) type. We certainly believe that this study will provide useful guidance for the development of novel inhibitors that are less susceptible to drug resistance.

Keywords: Paclitaxel; R306C & F270V Mutations; Molecular Docking; Molecular Dynamics.

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-ORA-09e

Tunable Signal Processing in Multi-site Phosphorylation Systems via Explicit Enzyme Activation

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ABSTRACT

Multi-site phosphorylation is a basic way of chemically encoding substrate function and a recurring feature of cell signalling pathways. It is a key control in many cellular processes and plays very important roles in many contexts, and dysregulation of this mechanism has been implicated in multiple diseases (including Alzheimer's disease)[1]. Numerous studies have explored information processing characteristics of multisite phosphorylation, through studies of the intrinsic kinetics[2,3,4]. Many of these studies focus on the module in isolation. In other words, all these studies conceptualize and deal with multi-site phosphorylation as the closed compartment of substrate and enzyme where reaction happens (similar to a reaction in a test tube). In this study, we build a bridge to connect the behaviour of multisite modification in isolation to that as part of pathways[5]. We study the effect of activation of the enzymes which is a basic way in which the module may be regulated. We find that these effects can induce multiple kinds of transitions, including to behaviour not seen intrinsically in the multisite modification module. We then build on these insights to investigate how these multi-site modification systems can be tuned by enzyme activation to realize a range of information processing outcomes for the design of synthetic phosphorylation circuits. Connecting the complexity of multi-site modification kinetics, with the pathways in which they are embedded, serves as a basis for teasing out many aspects of their interaction, providing insights of relevance in systems biology, synthetic biology/chemistry and chemical information processing.

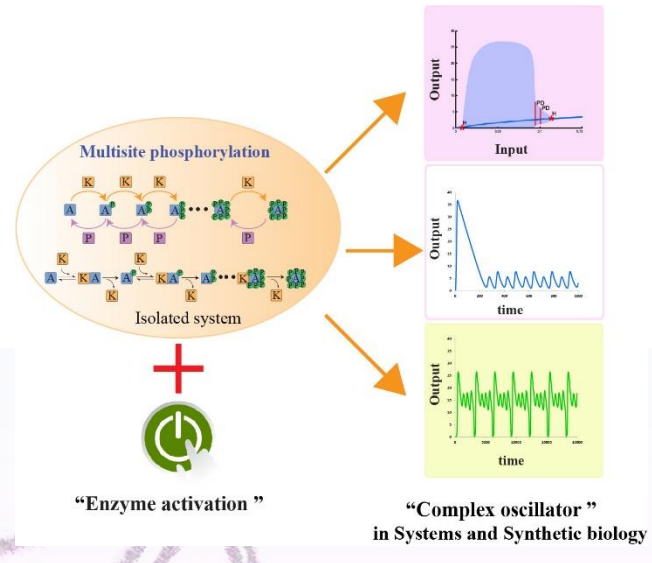

Figure 1. Oscillations induced by the presence of linear enzyme activation/inactivation. Multi-site modification systems can be tuned by simple enzyme activation to realize a range of information processing outcomes (such as period-doubling oscillations, mixed-mode oscillation) for the design of synthetic phosphorylation circuits. (image adapted from [4] and [5])

Keywords: Multisite Modification, Signalling Pathway, Information Processing, Enzyme Activation, Transitions, Dynamics, Oscillations, Regulation.

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In silico screening of chalcones against Epstein-Barr Nuclear Antigen 1 protein in Epstein-Barr virus.

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ABSTRACT

Epstein-Barr Virus (EBV) is the herpesvirus 4. EBV has induced changes to cell and best known as the cause of infectious mononucleosis and long-term EBV infections associated with higher risk cancer. During latent infection, EBV does express a limited set of viral gene products that promote host-cell survival and proliferation. The maintenance of the latent viral genome depends on the functions of the Epstein-Barr Nuclear Antigen 1 protein (EBNA1), which is essential for viral genome maintenance and for infected-cell survival. In this study, we aimed to screen chalcones, which can exhibit several biological activities. The EBNA1 structure was obtained from X-ray crystal structure in protein data bank (PDB), entry code 1B3T. Ligand-protein interactions were investigated using CDOCKER and Molecular Operating Environment docking program. All systems were performed by Molecular dynamic simulations using AMBER16 software package. The binding free energy of all complexes was evaluated by the MM/GBSA.py module. Based on the interaction energy, the compound group 3 showed the interaction energies lower than those of 4-hydroxyderricin. From MD simulation, the last 20-ns trajectories were extracted for analysis in terms of structure, dynamics and ligand-protein interactions as well as ligand-binding affinities based on the MM/GBSA methods. Interestingly compound 3a and 3b showed the strong binding affinity than those 4-hydroxyderricin.

	3a	3b	3d	3e	4-hydroxyderricin
ΔE_{vdw}	-43.2 ± 2.6	-31.2 ± 4.3	-33.2 ± 2.5	-35.4 ± 2.3	-38.2 ± 2.4
ΔE_{elec}	-4.4 ± 4.2	-15.5 ± 3.8	-13.3 ± 6.1	0.4 ± 4.8	-17.4 ± 4.9
ΔE_{MM}	-47.6 ± 4.8	-46.7 ± 3.9	-46.5 ± 6.2	-34.9 ± 5.4	-55.6 ± 4.8
ΔG_{polar}	22.5 ± 3.9	29.6 ± 2.9	31.2 ± 5.5	18.4 ± 4.1	36.2 ± 4.1
$\Delta G_{non\text{-}polar}$	-5.2 ± 0.3	-3.9 ± 0.5	-3.8 ± 0.2	-4.0 ± 0.2	-4.9 ± 0.2
ΔG_{sol}	17.3 ± 3.9	25.8 ± 2.9	27.4 ± 5.4	14.0 ± 4.0	31.2 ± 4.0
-TΔS	21.4 ± 6.4	13.5 ± 6.4	15.4 ± 10.3	20.6 ± 10.2	21.1 ± 14.0
ΔG_{bind}	-8.9	-7.4	-3.7	-0.3	-3.3

Figure 1. The binding free energy and energy components (kcal/mol) for 3a, 3b, 3d, 3e and 4-hydroxyderricin complexes predicted by the MM/GBSA method.

Keywords: Epstein-Barr Virus, Epstein-Barr Nuclear Antigen 1 protein, chalcones, Molecular Dynamics Simulation.

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In Silico Studies on Potential Compounds against Viral Hepatitis B Reverse Transcriptase

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ABSTRACT

Hepatitis B virus (HBV) is a small enveloped DNA virus, which attacks the human liver causing both acute and chronic diseases. Over 240 million people are infected with a consequence of more than 686,000 people death per year due to cirrhosis and liver cancer. Current therapeutic drugs use the nucleotide analogues (NUCs) as a competitive inhibitor against HBV reverse transcriptase (RT), an essential enzyme pivotally involved in viral replication. NUCs inhibits RT enzyme by interacting with the catalytic region containing four catalytic residues (YMDD) that is also found in the catalytic binding site of HIV-1 RT. In this study, we aimed to understand the ligand-protein interaction of known anti-HBV (lamivudine) and anti-HIV (stavudine, didanosine and zidovudine) drugs and to screen for more potent compounds against HBV RT using computational approaches. In addition, we also study the conformational change of HIV drugs in explicit solvent at different temperature. The 100-ns molecular dynamics (MD) simulations were performed on the HBV RT in complex with these four drugs in comparison to that of deoxythymidine triphosphate (dTTP) substrate. The predicted binding free energies show that the anti-HIV drug, stavudine, has the binding affinity against HBV RT in comparable with that of lamivudine and relatively better than the dTTP substrate. This finding suggests that the starvudine might able to inhibit this enzyme similar to the other anti-HIV drugs such as emtricitabine. To find new anti-HBV agents, the pharmacophore models generated from 4000 MD frames of substrate complex were used to screen for potentially effective compounds from DrugBank database using LigandScout program. Based on the following criterions, type of drug groups, pharmacophore-fit score and core structure, the three commercial drugs floxuridine, trifluridine and sofosbuvir were collected. In addition, the conformations of anti-HIV drugs in unbound state were studied by replica exchange MD simulations for comparison with those in bound state.

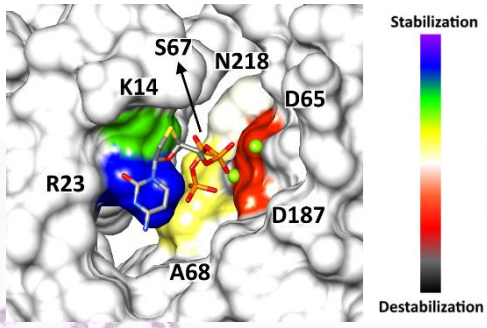

Figure 1. Per-residue decomposition free energy of HBV RT for lamivudine binding

Keywords: HBV reverse transcriptase, Molecular dynamics simulation, Virtual screening, Pharmacophore, Replica-exchange molecular dynamics

Binding investigation of pyrazine derivative against Glycogen synthase kinase-3 (GSK-3β) via in silico molecular dynamics simulations

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ABSTRACT

Glycogen synthase kinase-3 (GSK-3β) is a serine/threonine protein kinase which plays a role in the regulation of many function, such as metabolic, signaling and structure protein. GSK-3β leads to the cause of diabetes, bipolar disorders, cancer and Alzheimer's disease (AD). In AD disease, the over-activity or over-expression of GSK-3β accounts for memory loss, tau hyperphosphorylation, increased β-amyloid production which are characteristic hallmarks of the AD disease. To date, GSK-3β is interested to study as a new protein target in AD disease. In this work, the binding mode between GSK-3β and a pyrazine derivative is investigated using molecular dynamics (MD) simulations for 100 ns in GROMACs program and binding energy is also studied using Gaussian 09 program. Consequently, MD simulations reveal the stabilized complex structure and key amino acids after 10 ns.The conformations of 10-100 ns MD trajectories are further clustered based on their conformation. The first conformational cluster posed the highest contribution is selected for analyzing the binding interaction of pyrazine derivative. H-bonds to ILE62, LYS85, APS133 and VAL135 are found. The obtained results can help for development and design new compound against AD disease.

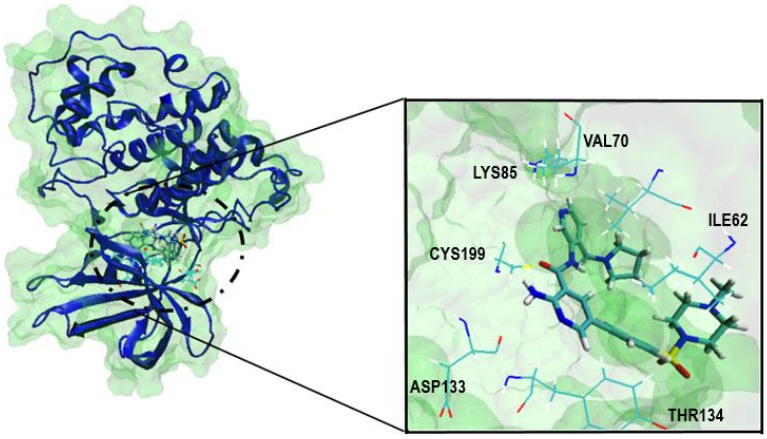

Figure 1. Structure of GSK-3β complexed with pyrazine derivative

Keywords: Alzheimer's disease (AD), Glycogen synthase kinase(GSK-3β), Molecular dynamics (MD) simulations, Pyrazine derivative

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Substrate binding mechanism of glycerophosphoethanolamine to glycerophosphodiesterase

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ABSTRACT

Glycogen synthase kinase-3 (GSK-3β) is a serine/threonine protein kinase which plays a role in the regulation of many function, such as metabolic, signaling and structure protein. GSK-3β leads to the cause of diabetes, bipolar disorders, cancer and Alzheimer's disease (AD). In AD disease, the over-activity or over-expression of GSK-3β accounts for memory loss, tau hyperphosphorylation, increased β-amyloid production which are characteristic hallmarks of the AD disease. To date, GSK-3β is interested to study as a new protein target in AD disease. In this work, the binding mode between GSK-3β and a pyrazine derivative is investigated using molecular dynamics (MD) simulations for 100 ns in GROMACs program and binding energy is also studied using Gaussian 09 program. Consequently, MD simulations reveal the stabilized complex structure and key amino acids after 10 ns.The conformations of 10-100 ns MD trajectories are further clustered based on their conformation. The first conformational cluster posed the highest contribution is selected for analyzing the binding interaction of pyrazine derivative. H-bonds to ILE62, LYS85, APS133 and VAL135 are found. The obtained results can help for development and design new compound against AD disease.

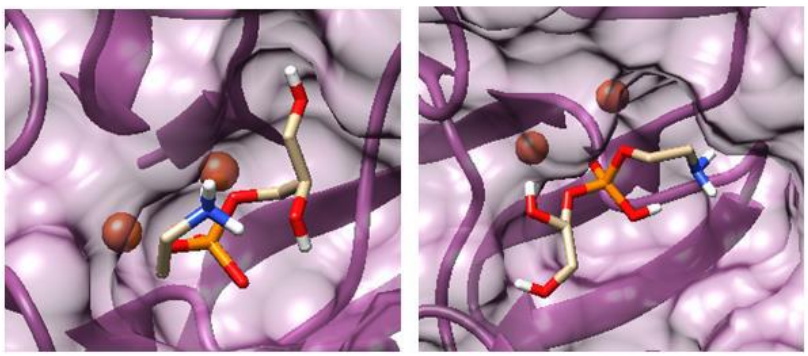

Figure 1. Docked structures of GPE substrate in both the forms in substrate binding pocket of active site of GpdQ

Homopharma-Based Identification Target of Phenolic Lipid Derivatives Against Dengue Virus Infected Cell

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ABSTRACT

Many compounds, similar to active inhibitors may bind to the same protein with similar interactions. This fact leads to the application of databases of drugs and other potent compounds. As these databases contain huge amounts of information from many different data sources, they are helpful tools in modern drug discovery. In the present study the dengue infection, caused by the dengue virus is investigated. No effective prevention or any therapeutic agent to cure this disease is known up to now. The secondary metabolites from cashew nut (*Anacardium occidentale*), anacardic acid, cardol and cardanol are phenolic lipid compounds with biological activities including anti-oxidant, anti-cancer, anti-inflammation, anti-microbial and anti-viral properties [1]. A Homopharma concept [2] was applied in this study in order to identify the possible protein targets for these phenolic lipid compounds. Using various databases almost 7000 similar structures were found starting from three known active substances based on 2D Tanimoto similarity (95%). A total of 1225 protein targets were selected from bioactivity analyses database, they were identified and clustered into 344 protein families, which were subsequently compared with dengue-host protein interactome. 31 overlapping human host proteins and one viral protein were used to evaluate the binding affinities by molecular docking of the phenolic lipid compounds. As a result, the NS5 protein was found to be a viral protein target for the considered phenolic lipids, and, thus, it could be a potential target for these compounds found by Homopharma-based identification target method. The reliability of this identification method has been verified by testing the known active compound and its protein target.

Homopharma-Based Identification Target of Phenolic Lipid Derivatives Against Dengue Virus Infected Cell

Kowit Hengphasatporn[1], Peter Wolschann[2,3] Jinn-Moon Yang[4,5*], Thanyada Rungrotmongkol[1,6C*]
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ABSTRACT

Computational-aided drug design (CADD) is the modern method to discovery the new drug or potent compound using published database which contains and collects information from many different data sources. Among of big data, many compounds similar to active or known inhibitors could bind to same protein family with similar interactions. The secondary metabolite from cashew nut (*Anacardium occidentale*); anacardic acid, cardol and cardanol are the phenolic lipid compounds that were reported their biological effects including anti-oxidant, anti-cancer, anti-inflammation, anti-microbial and anti-viral properties [1]. More than half the world's population had got high risk of dengue infection by dengue virus (DENV) through its vector however, there is no effective prevention or therapeutic agent to cure this infection. Homopharma concept was applied in this study in order to identify the possible protein targets of phenolic lipid compounds [2]. Almost 7,000 similar structures were searched from 3 known active compounds based on 2D Tanimoto similarity (95%). Using bioactivity analysis database, the 1,225 protein targets relevant to similar compounds were revealed. A total of 1,225 proteins were identified and clustered into 344 protein families that were then compared with dengue-host protein interactome. The 31 overlapped human host proteins and 1 viral protein from previous step were used to evaluated the binding affinity by molecular docking with these phenolic lipid compounds and compare the binding affinity with crystal ligand. As a result, the NS5 protein was found to be viral protein target for our focused phenolic lipids and thus it could be the potential target of these compounds based on homopharma-based identification target method. The reliability of this identification method has verified by the known active compound and its protein target.

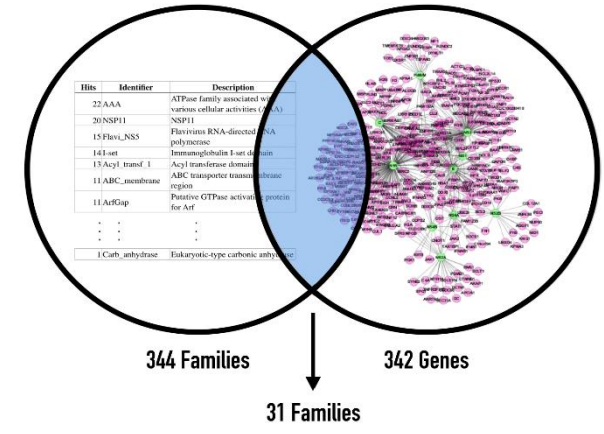

Figure 1. An example figure or table.

Keywords: Computational biology, Dengue, Homopharma, Target identification

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Computational Biology, Bioinformatics, Biochemistry and Biophysics
BIO-POS-07

Molecular Dynamics Study on Human Serine Hydroxymethyltransferase with Pyridoxal Phosphate Bound

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ABSTRACT

Serine hydroxymethyltransferase (SHMT), a pyridoxal phosphate (PLP; vitamin B6) dependent enzyme, plays an important role in cellular one carbon pathways by catalysing the reversible, simultaneous conversions of L-serine to glycine and tetrahydrofolate (THF) to 5,10-methylenetetrahydrofolate (5,10-CH2-THF), a requisite precursor for DNA/RNA biosynthesis. In order to understand the structures and dynamics of wild-type and deflapped human SHMT strains with PLP bound, the apo-dimeric and tetrameric enzymes with and without PLP were performed by molecular dynamics (MD) simulation. As a result, the apo-dimeric and tetrameric wild type and deflapped forms (without PLP) are more flexible than holo-dimeric and tetrameric wild type and deflapped form (with PLP), since the holoenzymes have structure integrity and stabilization. In comparison between wild type and deflapped enzymes, while overall protein has relatively similar fluctuation, the flap motif in wild type shows high flexibility because it is fully solvated by waters. The binding of PLP in tetrameric and dimer forms could enhance the protein stability. The obtained information provides a clear picture of PLP cofactor binding to human SHMT.

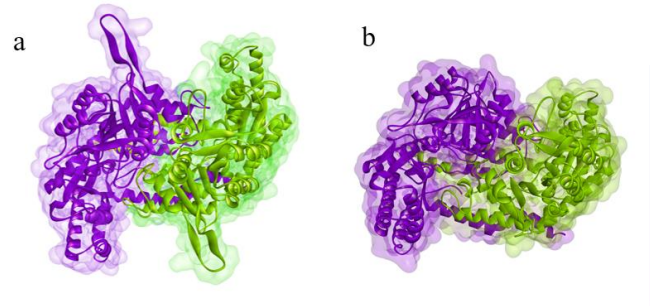

Figure 1. Structures of serine hydroxymethyltransferase in (a) wild type and (b) deflapped dimeric forms.

Keywords: Serine hydroxymethyltransferase, Structure integrity, Stabilization, Pyridoxal phosphate, Molecular dynamics simulation

Effect of phenolic compounds as H5N1 influenza A neuraminidase inhibitors by molecular dynamic simulation

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ABSTRACT

As worldwide epidemic strains, influenza A (H5N1) caused acute respiratory diseases in human. Neuraminidase, a membrane-bound glycoprotein, plays a dominant role in the viral life cycle and thus is one of the particular potential targets for novel antiviral therapeutics. This work aimed to study the 4 phenolic compound (caffeic acid (CA), Rosmarinic acid (RA) and 2 unknown phenolic compounds (NA1, NA2)) act as anti-influenza agents by computational techniques. The structure was obtained from crystal structure in protein data bank (PDB), entry code 2HU4. Ligand-protein interactions were investigated using CHARMM based docking software (CDOCKER) of the Discovery Studio 2.5 (Accelrys Inc., San Diego, CA, USA) suite of program. Each docked complex with lowest interaction energy was chosen for molecular dynamics study using AMBER16 software package. All structures and dynamics properties were computed by the cpptraj module, while the binding free energy of complex was evaluated by the MMGBSA.py module. The obtained results suggest that RA has the lowest interaction energy (-15.62 kcal/mol) and binds with the four important residues Arg118, Arg151, Arg152 and Ser256 of neuraminidase. In addition, this compound experimentally shows inhibitory activity with IC50 value of -0.39 μM.

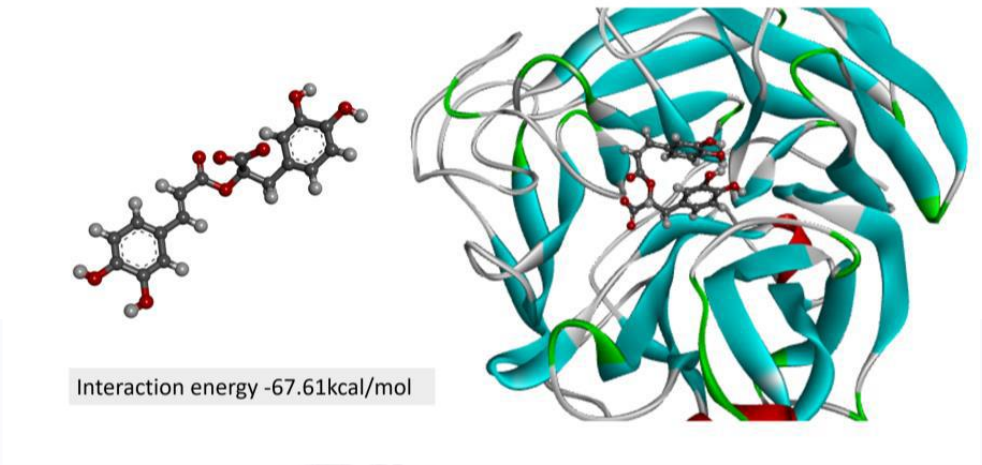

Figure 1. Docked structure of RA/neuraminidase complex

Keywords: Phenolic compounds, H5N1 avian flu, Molecular docking, Molecular dynamics simulation

II) Computational Chemistry

Mechanistic Insights into Metal-Catalyzed Highly Selective Organic Transformation Reactions

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ABSTRACT

Modern density functional theory is very useful to analyze mechanistic insights into metal-catalyzed highly-selective conversion reactions. Rh(I)BINAP-catalyzed isomerization of allylic amines was examined by using DFT, QM/MM calculations, and the Artificial Force Induced Reaction (AFIR) method, which enables us to perform automatic reaction pathway search. [1] Graph theory approach for this complicated reaction pathways by using Prim's algorithm is very useful to find the most economical reaction pathway. The dissociative mechanisms which do not involve two allylic amine molecules are preferred over the associative mechanisms, which was proposed by previous model studies by ab initio and DFT calculations. We also reported DFT studies on Ni-catalyzed Suzuki-Miyaura coupling through C−O bond activations of methoxynaphthalene with phenyl boronic acid. [2] This reaction goes through rate-determining oxidative addition of the C−O bond followed by transmetalation and reductive elimination to lead a coupling product. Electron donating nature of the ICy N-heterocyclic (NHC) carbene ligand makes the activation energy of the oxidative addition more feasible. In addition to those studies, importance of non-covalent interaction on second-sphere coordination of indole group on one-electron oxidized Cu(II)-salen complexes [3] and origin of high enantioselectivity in Cu(I)-catalyzed alkynylation of a-ketoester. In the latter studies, interactions between a cyclohexyl group of the a-ketoester and cyclohexylphosphine were found. [4]

Keywords: DFT calculations, homogeneous metal catalyst, reaction mechanisms

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Seiji Mori was born in Tokyo, Japan and obtained his PhD degree from the University of Tokyo under guidance of Prof. Eiichi Nakamura in 1998. After working in Emory University, USA with Prof. Keiji Morokuma and Kyoto University, he becomes an assistant professor (2000-2001), associate professor (2001-2012) and full professor (2012-) at Ibaraki University, Japan. He was appointed as an assistant vice president for international strategy of Ibaraki University between 2015-2017.8080

Towards a Molecular Understanding of the Relative Reactivities of ?-Caprolactone and L-Lactide in Their Homo- and Copolymerization Using Aluminium Salen-type Initiators: A DFT Study

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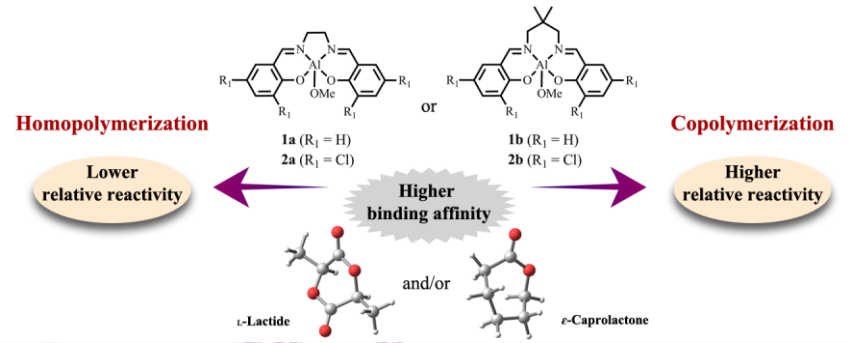
ABSTRACT

Polylactide (PLA), poly(ε-caprolactone) (PCL), and their copolymers have been widely synthesized and investigated for their medical applications due to their biodegradability and other biocompatible properties. In most catalytic homopolymerization systems, the polymerization rate of ε-caprolactone (ε-CL) is found to be substantially higher than that of L-lactide (L-LA). However, a reversed order in the relative reactivities of ε-CL and L-LA seems to be a common feature found in the copolymerization systems. To provide a consensus on the most plausible explanation of this phenomenon, the initiation and first propagation steps of the ring-opening polymerization (ROP) of ε-CL and L-LA mediated by aluminium salen-type initiators were investigated at the molecular level using density functional theory (DFT). The results show that, even though the apparent ROP mechanisms are similar for all systems studied, the activation barriers for the rate-limiting transition states are different and depend on the initiator. The relative reactivities of the initiators toward the ROP of the two monomers are predicted to be in good agreement with experimentally and theoretically observed trends for systems with different bridging units and electronic properties of the ligand substituents. However, this does not entail similar reactivities in all polymerization processes. An explanation for this, here the different reactivities observed for homo- and copolymerization (for the two types of monomers) is found in their different binding affinities with the propagating active species. Several experimentally observed features, such as e.g. reaction rates, in other related homopolymerization and random copolymerization systems with these two monomers can also be rationalized.



Keywords: L-Lactide, ε-Caprolactone, Salen-aluminium, Ring-opening polymerization, DFT

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Tanin Nanok received his Ph.D. degrees in Chemistry and in Physical Chemistry under a cotutelle doctoral program between Kasetsart University (Thailand) and the University of Bordeaux 1 (France) in 2005. He has started a faculty position at Kasetsart University since 2006 and left for his postdoctoral research at the Institute for Theoretical Physics of the University of Leipzig (Germany) in 2008 before returning to Kasetsart University to continue his academic career in 2009. His current research interests are focused on computational studies of organic reactions catalyzed by zeolites and organometallic complexes.

QSAR Study of Phenoxy-imine Catalytic Behavior in Polyethylene Polymerization

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ABSTRACT

A quantitative structure activity relationship (QSAR) of Ti-phenoxy-imine based catalysts (Figure 1a) was investigated to clarify the role of structural properties of catalysts in polyethylene polymerization activity. The steric and electronic properties of the FI-Ti catalysts were analyzed based on the density functional theory (DFT) with M06L/6-31G** and LANL2DZ basis functions. The QSAR equation with genetic algorithm analysis showed that catalytic activity mainly depended on HOMO energy level (X1) and total charge of the **R3** substituent group (X2) which was connected to phenyl next to imine group. The QSAR model showed a good R^2 value of 0.997 and highly reliable activity predication with cross validation R^2 (R^2_{cv}) value of 0.927. Designed criteria is the concept of "Head-Hat" which mean to keep the phenoxy-imine derivatives, and then changes the transition metals. In this work, all Ti-phenoxy-imine catalysts, the Ti metal was replaced by Zr or Ni as metal center atom. All new designed catalysts were built and optimized to extract the X1 and X2 properties. Consequently, their polyethylene polymerization activities were predicted based on the Ti-phenoxy-imine QSAR equation. All predicted activities (kg(PE)/mol·cat·MPa·h) of Ti-, Zr- and Ni-phenoxy-imine catalysts were plotted, and the results found that the new complexes from post metallocenes with Ni complexes trend to increase catalytic activity than that of Zr complexes. Therefore, the DFT calculation and QSAR technique are useful methods for studying on molecular design or catalysts' screening which are beneficial for industrial researches.

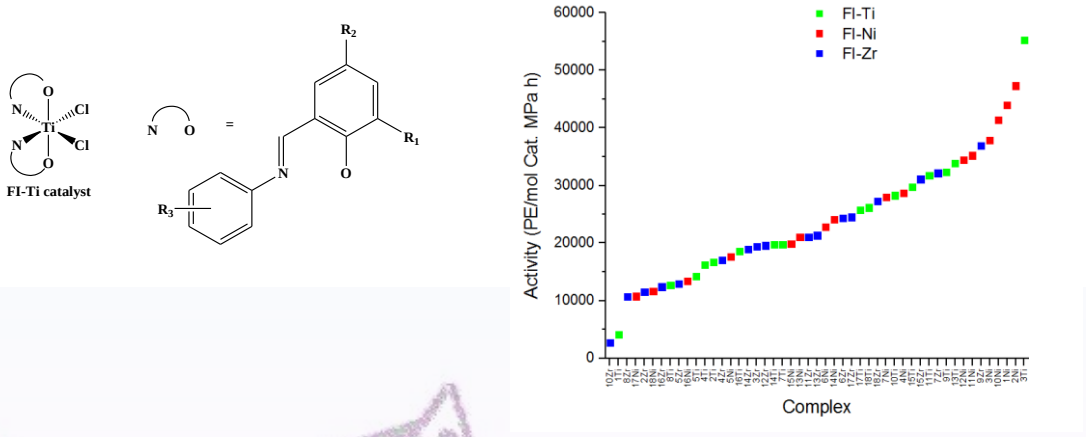

Figure 1. Ti-phenoxy-imine template (a) and predicted kg(PE) activities of Ti-, Ni-, and Zr-phenoxy-imine based catalysts (b)

Keywords: Phenoxy-imine, Ethylene polymerization, QSAR, DFT

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Research Interests

• Theoretical researches on reaction mechanism investigations, such N_2O-, H_2S-decompositions, NH_3-SCR of NO, Etc.
• Structural and electronic investigations on various types of catalysts and inhibitors.
• An application of quantitative structure activity (or property) relationship (QSAR, QSPR) on both biological inhibitors and petroleum catalysts Contact ：

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2011.10 – 2014.4, Shanghai University, Postdoctoral researcher
2009.1 – 2011.9, Kasetsart University, Postdoctoral researcher
2005.6 - 2008.4, Kasetsart University, PhD student.

Her researches on theoretical researches on reaction mechanism investigations, such N_2O-, H_2S-decompositions, NH_3-SCR of NO were supported by the National Natural Science Foundation of China (NSFC) and the Science and Technology Commission of Shanghai Municipality (STCSM). She has published the publications in EST, CST, JPCC, etc which were cited more than 555 times (without self-citations) and her current H-index is 11 (Web of Science Ref, 2018.5.15)

The Imprint of Electronic Structure on the Reactivity of Linear Carbon Chain Cations

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ABSTRACT

Due to the flexible balance of s and p orbitals, carbon species are found in many different geometrical forms: linear chains, planar graphene, and three dimensional fullerenes. Furthermore, in the astrophysics and combustion communities, many studies have been performed on carbon clusters with a focus on the effect of geometric structure towards the reactivity. Although there have been a lot of studies on these clusters, an understanding of their fairly complex electronic states is still lacking. Here we thus investigate the reactions of size and isomer selected carbon cations C_n + (*n* = 4–9) and D_2 with an emphasis on the imprint of electronic structure on reactivity

Only linear C_nD^+ products were observed for the odd (*n* = 5, 7, 9) linear clusters, while $C_nD_2^+$ was the main product for the even clusters. For the reaction rate constants determined for these two channels, we obtained the following two features: (1) the rate constant decreases with the size *n*, and (2) even-sized clusters have lower rate constants than neighboring odd-sized clusters. In the theoretical calculations using the CCSD(T) and B3LYP methods with the cc-pVTZ basis, we found that a low lying $^2\Sigma$ state in odd clusters may play an important role in these reactions. The existence of this lower energy $^2\Sigma$ state opposes the previous interpretation that the $^2\Pi_{g/u}$ state is the dominant electronic state for linear C_n + (*n* = 4–9) clusters. We showed that a barrierless radical abstraction forming C_nD^+ occurs through a direct head on approach for the $^2\Sigma$ state C_n^+. In contrast, a carbene-like insertion forming $C_nD_2^+$ occurs through a sideways approach for the $^2\Pi_{g/u}$ state C_n^+. We have concluded that the higher rate constants for the odd clusters come from the existence of symmetry broken $^2\Sigma$ states which are absent in even linear clusters.

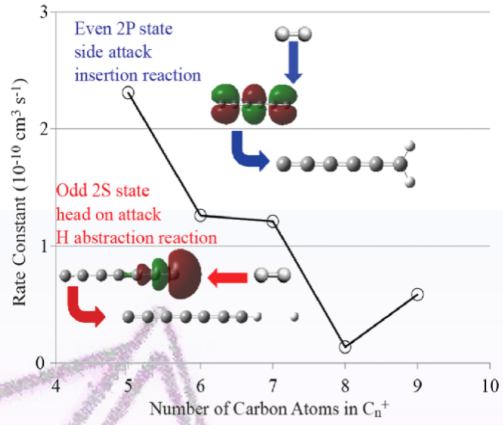

Figure Experimental Reaction rate of the carbon chain length dependence of the $C_n^+ + H_2$ reaction

Keywords: carbon cluster, electronic structure

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Kaito Takahashi is a Japanese theoretical chemist working as an associate research fellow at the Institute of Atomic and Molecular Sciences, Academia Sinica (IAMS, AS) Taiwan. In 2005, he obtained his Ph.D. from Keio University under the tutelage of Prof. Satoshi Yabushita. After four years of postdoctoral fellow research under Prof. Rex. T. Skojde, he started his lab at IAMS in 2009. His scientific interest for the past few years has been to theoretically understand properties that control reactions and to simulate vibrational, photodetachment, and X-ray absorption spectra. In 2017, he received the Academia Sinica Career Development Award for his theoretical studies on Criegee intermediates.

Theoretical Investigation of CO_2 Electrochemical Reduction on Cu-based Catalysts: The Effect of Surface Facets and The Role of S Dopant

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ABSTRACT

Electrochemical reduction of CO_2 is a promising process which can reduce carbon footprint and bring us toward future neutral CO_2 cycle. The process is enable conversion of waste CO_2 to various valuable hydrocarbon fuels and chemicals using low energy supply which can be provided by renewable energy resources such as solar cells. Copper is known to catalyze CO_2 electroreduction best compared to other pure metals. Recently, extensive researches have been exploring alternatives for catalyst design to increase selectivity and reactivity of CO_2 electrochemical reduction. In this work, we aim to understand the fundamental toward improving catalytic selectivity of Cu-based catalysts towards formate and C_2 species (i.e. ethylene) production.

The copper surface facet is one of the crucial factor to promote hydrocarbon C_2 species production. The study focused on Cu(100), Cu(110) and Cu(111) surfaces. The production of ethylene showed higher activity and selectivity on Cu(100) surface compared to that on Cu(110) and Cu(111) surfaces. Here, we applied density functional theory (DFT) calculations to demonstrate a buildup of high CO adsorption coverage to have a significant impact on lowering energy barrier for CO-CO coupling which lead to C_2 species formation. The high CO adsorption coverage on Cu(100) surface can best facilitate the CO-CO coupling reaction showing the lowest energy barrier.

Furthermore, the calculations describe the mechanistic workings of CuS catalyst that can reduce CO_2 to formate with a remarkable faradaic efficiency of 75% and current density found in the experiments. The *COOH and HCOO* are the key intermediates which determine the selective CO* and formate production, respectively. The results demonstrate that the presence of sulfur on copper surfaces can modify the bindings between the Cu atoms and adsorbed *COOH and HCOO* intermediates at high coverages, such that the formation of *COOH toward CO is suppressed while the formation of HCOO* towards formate is favored.

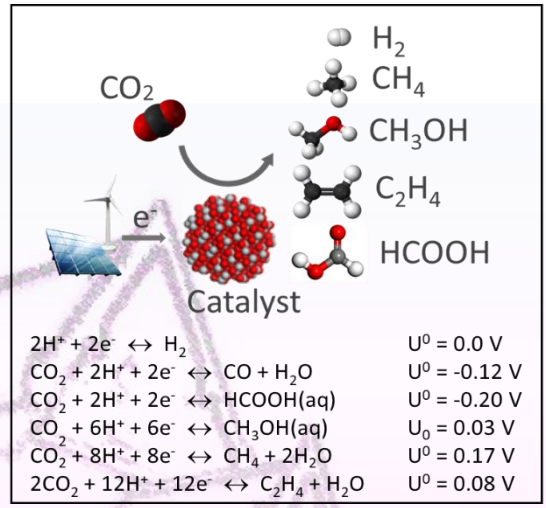

Figure CO_2 electroreduction reactions.

Keywords: CO_2 electroreduction, Denstity Functional Theory, heterogeneous catalyst.

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3. P. Hirunsit*, J. Phys. Chem. C, 2013. 117(16): p. 8262-8268.

Pussana Hirunsit is a researcher at Nanoscale Simulation Laboratory, National Nanotechnology Center (NANOTEC), Thailand since 2012. In 2010, she received her Ph.D in chemical engineering from Texas A&M University, USA. During 2010-2012, she joined Center for Nanoscale Materials (CNM) at Argonne National Laboratory, USA as a postdoctoral appointee.

Her research interest is to apply first principle calculations and molecular dynamic simulations to determine structural, kinetic, thermodynamic, and electronic properties of heterogeneous catalysis at the atomic scale and nanostructured materials leading to the fundamental development of novel catalysts and energy-related nanostructured materials, particularly metal, metal oxides and carbon-based materials that are designed to tailor properties. She is focusing on the following research topics;

- Electrocatalysts for CO_2 electrochemical conversion to chemicals and fuels
- Catalysis on metal and metal oxides surfaces for conversion of biomass-derived oxygenated feedstocks to value-added chemicals and fuels
- Carbon-based nanostructured materials for batteries and supercapacitors
- Solid-electrolyte interface phenomena

Application of Computational Methods in Anti-malarial Drug Discovery

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ABSTRACT

This talk details the theoretical and experimental efforts we have undertaken with the aim of developing new treatments targeting the Plasmodium falciparum (Pf) parasite, a key cause of malaria worldwide. We describe our efforts to develop inhibitors targeting protein kinases as a means to eradicate the Pf parasite. Seventeen new 2,4 diamino-pyrimidines analogs were designed, synthesized and tested against the resistant K1 strain of Pf and normal mammalian cells leading to compounds with comparable anti-malarial activity as the drug Chloroquine. We also describe our theoretical studies to elucidate the biochemical mechanism of Dihydropteroate synthase DHPS, a validated anti-malarial target whose efficacy in treating malaria is being increasingly challenged as a result of disease-based mutations. To date no detailed computational analysis of the protein mechanism has been made. We have employed hybrid QM/MM calculations to assess the energetics associated with S_N1 and S_N2 processes, identify whether the S_N1 process involves a carbocation or neutral DHP intermediate, uncover the identity of the general base in the catalytic mechanism, and understand the differences in substrate *vs.* inhibitor reactivity.

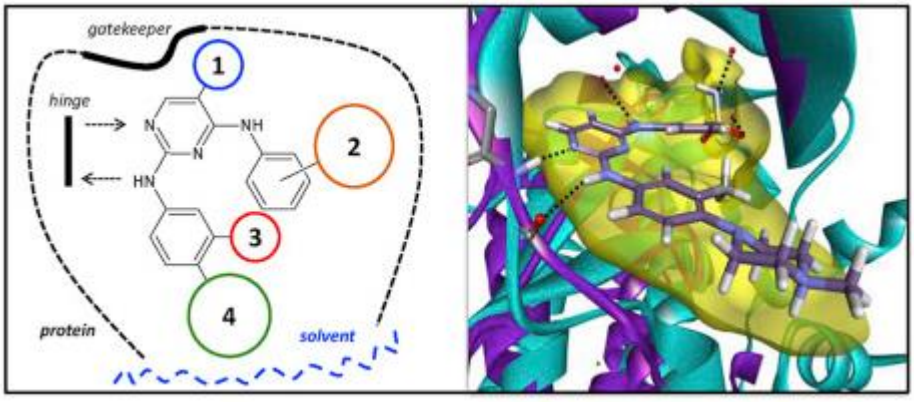

Figure An example figure or table.

Keywords: malaria, medicinal chemistry, QM/MM, DHPS, protein kinase.

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Significance of Urea-Aromatic Interactions in Biology: A Computational Study

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ABSTRACT

Urea is a chemical denaturant that assists protein unfolding and shifts the folding equilibrium towards the unfolded state. While a number of studies that attempted to understand the molecular mechanism of this phenomenon have been reported during the last three decades, a general consensus is lacking. It has been experimentally shown that among all the functional groups in proteins, urea interacts strongly with the aromatic groups. The nature of the interactions between urea and aromatic groups which makes it more stable than those involving urea and polar groups was not understood. The presentation will discuss our attempts at providing structural, thermodynamic and kinetic basis of these novel interactions. Free energy calculations on the unfolding of Trp-cage miniprotein reveal the importance of urea-aromatic interactions in the unfolding process. The primary mode of interaction between the two is shown to be stacking interactions in addition to hydrogen bonded and NH-π interactions.[1] This was further quantified by thermodynamic integration and quantum mechanical calculations. Lifetime calculations based on μs long MD simulations reveal these to be long lasting in the ps timescales.

We further show that stacking type interactions between urea and aromatic groups have significant role to play in urea transporters, damaged DNA with urea lesions and in drug-receptor interactions. All the three structures of urea transporters that have been solved so far, aromatic residues line the selectivity pore of the channel. We show using umbrella sampling free energy calculations that favourable urea-aromatic interactions are directly responsible for the ability of these transporters to discriminate from other molecules for transport across cell membranes.[2] Such stacking interactions lower the barrier for the transportation of urea (compared to other molecules) to pass through the selectivity filter.

DNA damage is a process by which the nucleobases are chemically modified which lead to hostile repercussions. One of the most common damage, thymine glycol has been shown to sometimes undergo hydrolysis to form urea moiety in the DNA. We show that such DNA molecules with such urea lesions are able to maintain their structural integrity because of their ability to form hydrogen bonding and stacking interactions just like the nucleobases.[3] We will also present a database analysis of all protein structures to which urea or urea derivatives are bound from the protein databank. It is found that statistically significant number of instances where urea and one of the aromatic amino acid side chains are involved in stacking interaction. In summary, we will present the role of novel and unusual stacking interaction between urea and aromatic in different facets in biology and the possible role of these interactions in increasing the binding affinity/specificity of drug-receptor interactions.

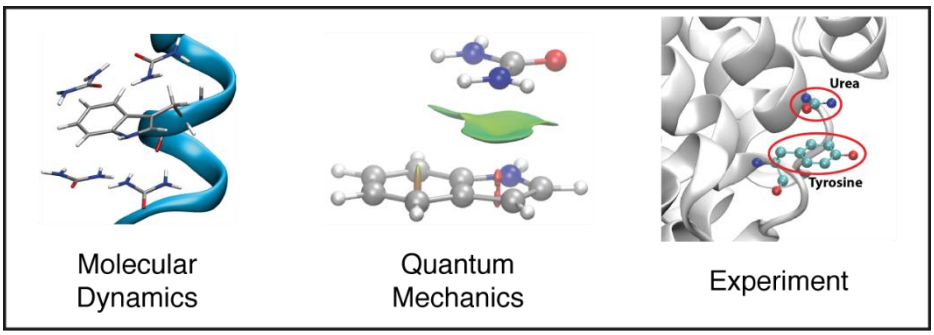

Figure Evidences for urea-aromatic stacking interactions from molecular dynamics simulations, high level quantum mechanical calculations and experimental structures.

Keywords: Protein folding, osmolytes, transporter proteins, damaged DNA.

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Deva obtained PhD in computational chemistry in 2004. After a postdoctoral fellowship in University of Maryland, he has been a faculty member in the IIIT Hyderabad. He is currently an Associate Professor and heads CCNSB. His research interests are in computational chemistry/biology. He is a recipient of Young scientist medal from the Indian National Science Academy, Innovative Young Biotechnologist award, and AICTE Career Award for Young Teachers.

Designing Efficient Nanoporous Catalysts for Industrial Chemical Reactions

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ABSTRACT

Chemical Reactions have been of essence in synthetic processes at the industrial level. It is commonly accomplished using nanoporous catalysts such as zeolites and metal-organic frameworks. Herein, we employ quantum chemical calculations to design the nanoporous catalysts with enhanced effectiveness for the chemical reactions such as propylene epoxidation, furfural hydrogenation and carbon monoxide oxidation. We first validate the nanoporous materials models with several cluster sizes to discover the suitable ones. We further investigate the mechanisms of these reactions to predict the favored reaction pathways occurred inside the nanoporous catalysts. Such calculations provide the activation energies and the rate-determining step of the reactions. Finally, we try to obtain informative chemical descriptors to predict the rate-determining step activation barriers to be used to rapidly screen promising catalysts for particular reactions.

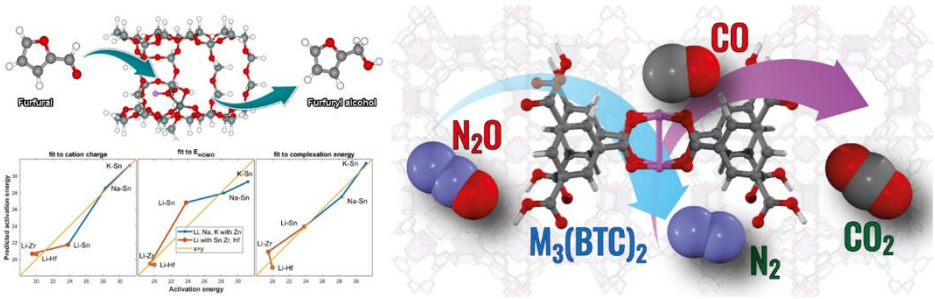

Figure 1. The studied industrial chemical reactions over nanoporous acidic catalysts.

Keywords: Quantum chemical calculation, Chemical reactions, Nanoporous catalysts, Chemical descriptors.

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Thana is currently a Lecturer in Chemistry at the Department of Chemistry, Faculty of Liberal Arts and Science, Kasetsart University, Kamphaeng Saen Campus. He received his Ph.D. degree from Department of Chemistry, Kasetsart University under Prof. Jumras Limtrakul. His current research activity is in the field of computational catalysis.

Computational Chemistry
CHE-INV-09

Temperature and Gas Loading Induced Structural-Dynamics Properties of Zeolitic Imidazolate Framework-90

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ABSTRACT

The effects of temperature and number of gas molecules in ZIF-90 were studied by using Gibbs Ensemble Monte Carlo (GEMC) simulations and Molecular Dynamics (MD) simulations. The adsorption and diffusion coefficients resulting from single gases, H2, CH4 and CO2, and H2/CH4 mixture are expected to yield information i.e. structural and dynamics properties. In this work we found the optimal parameter set between gas molecules and ZIF-90 framework as proved by adsorption isotherm calculations when compared with experimental data. Interestingly, the structural change namely gate opening in ZIF-90 appeared only at high temperatures under loading with H2, CH4 molecules and H2/CH4 mixture. For CO2 molecules, the gate opening appeared caused by both temperature and number of CO2 molecules loading as well. The preferential adsorption site for all gas molecules is located at the organic linker of ZIF-90. The diffusion coefficient shows high mobility at high temperature while adsorption in ZIF-90 is low for all gas molecules at high temperature. Also an increase of the membrane selectivity by increased temperature could be found for H2/CH4 mixture.

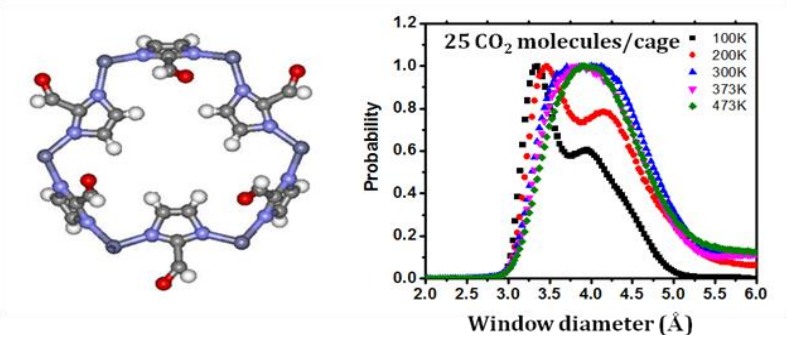

Figure1. The window diameters of ZIF-90 when loading 25 CO_2 molecules/cage.

Keywords: Gate Opening, Adsorption, Diffusion, ZIF-90, MD and GEMC Simulations

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A theoretical study of fluorene based copolymers for solar cell applications

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ABSTRACT

The structural, electronic, and charge properties of fluorine polymer (FF)n and fluorine copolymers (FX)n (X = Furan (Fu), Pyrrole (Py), Phosphor (Phos), and Para-Phenylene Vinylene (PPV), n = 1-4 repeating unit) were studied using the B3LYP/6-31G(d) method. As the result of structural properties, (FPPV)4 copolymer shows the planar structure with the dihedral angles close to 180 degree, corresponding to the smallest band gap of 2.69 eV. In contrast, the (FF)4 and (FX)4 structures, when X = Fu, Py, Phos, predict the band gap values spanning in the range of 2.78-3.53 eV, reflecting the capacity for light absorption in a wide range. For all (FX)4 copolymers the reorganization energies of hole (λh) are smaller than those of electron (λe), indicating better efficiency of hole mobility. As compared to others, the structure of (FPPV)4 copolymers gives lower value of reorganization energy of hole (λh). This means that conducting copolymer between fluorene (F) and para-polyphenylene vinylene (PPV) helps to improve charge carrier transfer rate. Our results demonstrate that the (FPPV)4 copolymers structure is a candidate for polymer solar cell application as donor materials.

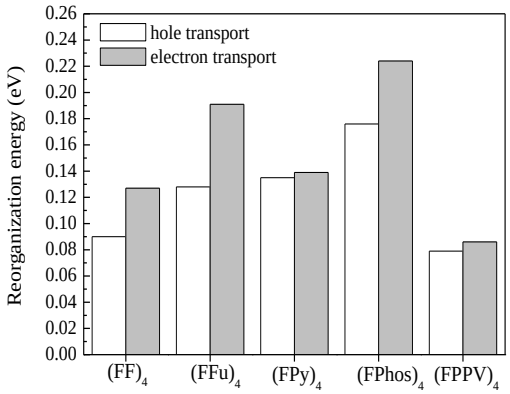

Figure 1. Reorganization energy for hole and electron of $(FF)_4$ and $(FX)_4$ (X = Fu, Py, Phos, and PPV) copolymers obtained by the B3LYP/6-31G(d) method.

Keywords: Band gap; Copolymer; DFT; Fluorenes; Reorganization energy

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Molecular Engineering of D-A Featured Organic Indole Sensitizers for Improving Performance Efficiency of Dye-Sensitized Solar Cells

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ABSTRACT

The electronic structures and photophysical properties of Indole dye forming D-A system as photosensitizes in dye-sensitized solar cells (DSSCs) were investigated. The ground-state structures of all molecules were fully optimized using density functional theory (DFT) at B3LYP/6-31g(d,p) level. The electronic absorption (λ_{abs}) of dye molecules was computed using time-dependent density functional theory (TDDFT) at CAM-B3LYP/6-31g(d,p) level. The solvation effect for dichloromethane was included by means of conductor-like polarizable continuum model (C-PCM). The effect of substitution position of anchoring groups on Indole ring was studied. We found that the substitution position of anchoring groups on Indole ring affected the absorption spectra of the dyes. These results indicate that the six-membered benzene ring influences on the red-shift of the dyes more than the five-membered nitrogen-containing pyrrole ring. The frontier molecular orbital results indicated that the intramolecular charge transfer (ICT) was occurred. Moreover we performed the adsorption of these dyes on the TiO_2 surface and the electron injection mechanisms were also investigated using a dye-$(TiO_2)_{38}$ cluster model, employing PBE and TD-CAM-B3LYP calculations. Our calculation results can provide useful information for improving an efficiency of new Indole dyes for DSSCs applications.

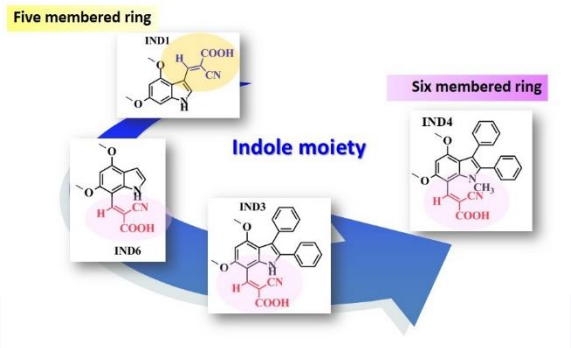

Figure 1. Sketch map of the synthesized Indole derivatives sensitizers.

Keywords: Dye sensitized solar cell, Indole derivatives, Density functional theory**.**

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Charge Carriers Distribution in Platinum Doped Graphitic Carbon Nitride Quantum Dot

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ABSTRACT

A novel graphitic carbon nitride has attracted broad attention from several areas of applications such as sensor, adsorbent, and photocatalyst. It possesses outstanding chemical and thermal stability, and it is environment friendly with biocompatibility and with low toxicity. In photoexcitation process, the photogenerated electron–hole pairs often recombine back to the ground state which is a weakness of using just g-C3N4 materials alone. In this work, we demonstrated the facilitation of platinum metal doping on the g-C3N4 quantum dot in photocatalytic process. Density functional theory was used to study on a model of 6 tri-s-triazine units (C36N52H12) built to represent g-C3N4 quantum dot. Geometry optimizations were carried out by using M06L functional with the 6-31G(d) basis set. Platinum atom treated by LANL2DZ Effective core potentials and basis set was placed among different sites on the g-C3N4 quantum dot model. Photoexcitation process was investigated by means of time-dependent density functional theory (TD-DFT) with a long-range (LR) corrected hybrid functional CAM-B3LYP and 6-31G(d) basis set was used. Atomic charges fitted to reproduce the electrostatic potential according to the Merz-Singh-Kollman scheme were selected to discuss. It was found that the pristine g-C3N4 QD structure is not arrange in a smooth horizontal plane due to the electrostatic repulsion between lone orbitals among adjacent tri-s-triazine units. This makes the g-C3N4 QD unconstrained to be doped with the Pt metal atom. The most stable position for Pt atom to anchor is on the window space and two crucial ligand-metal interactions detected between nitrogen atom in tri-s-triazine and Pt atom. Pt atom holds positively charge at +0.270e. The adsorption energy between Pt atom and g-C3N4 QD is calculated to be -52.58 kcal/mol. The calculated LUMO-HOMO energy gap for the g-C3N4 QD 6.21 eV which is very large while the value for Pt doped g-C3N4 is 3.30 eV. The density distributions of hole, electron and density difference between electron and hole were conducted to see the diffusion of those charge carries in both systems. The excited electron and hole of g-C3N4 QD are widely dispersed among the whole system. It should be noticed that hole is commonly localized on nitrogen atoms in tri-s-triazine units while electron is shifted to nearby carbon atoms. This observation might infer to the electron-hole charge recombination found in the pristine g-C3N4 QD. In Pt doped g-C3N4 QD, the excited electron is localized near Pt atom while the hole density is commonly found around anchoring area between Pt and connected tri-s-triazine groups. Accordingly, the region should be active site for desired photo-redox reactions. Our finding might endorse the initiative of using metal doping for improve the catalytic performance of the g-C3N4 materials.

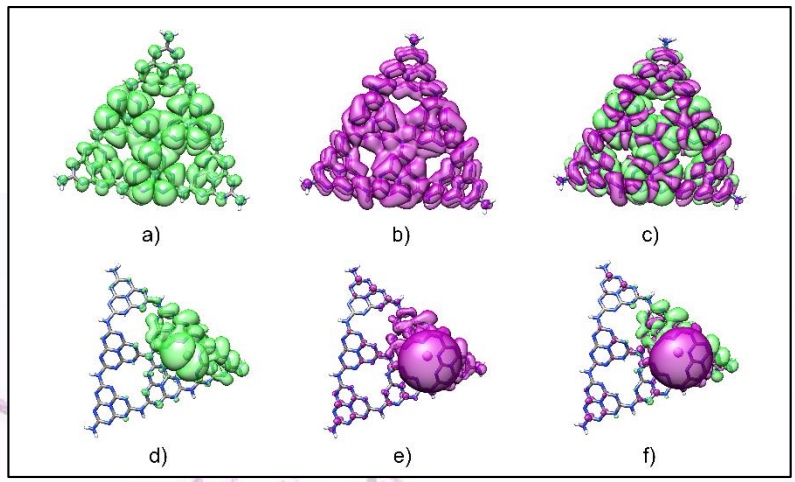

Figure 1. Hole (a), electron (b) and charge density difference (c) distribution in pristine g-C_3N_4 are shown in comparison with hole (d), electron (e) and charge density difference (f) distribution in Pt doped g-C_3N_4 (isovalue = 1.0 x 10^{-4} e/A^3)

Keywords: g-C3N4, photoexcitation, electron-hole charge recombination, charge separation.

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The mechanism of carbon dioxide hydrogenation to formic acid on Pt-boron nitride nanosheets (Pt-BNNSs): A DFT study

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ABSTRACT

The catalytic conversion of CO_2 to valuable chemicals such as formic acid, formaldehyde and methanol has received much attention from industrial sector. In the present work, the reaction mechanism of CO_2 hydrogenation to formic acid on Pt-doped boron nitride nanosheets (Pt-BNNS) and Pt-boron-vacancy (Pt-BV) have been investigated by means of the density functional theory (DFT). Two possible reaction mechanisms were proposed, namely concerted and stepwise mechanism. Our results found that the stepwise mechanism are more favorable. In the stepwise mechanism, the formic acid can occur via carboxylate intermediate (COOH) with the activation barrier for the rate-determining step of this mechanism is 0.78 eV. The calculation results provide the basis for exploring the Pt-BV catalysts in the hydrogenation of CO_2 involved in the greenhouse gas reduction, and the conversion of greenhouse gases.

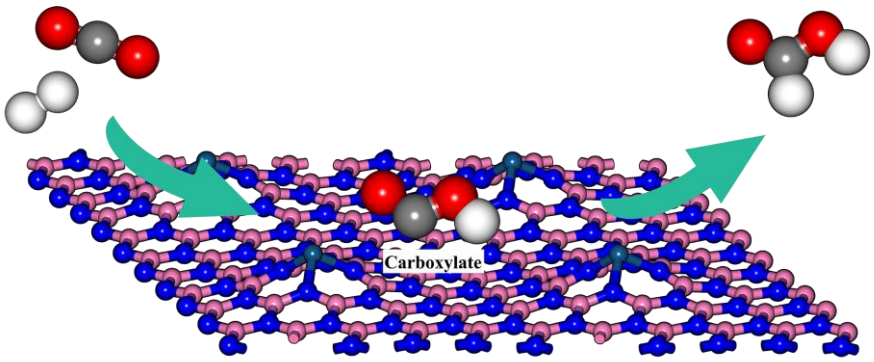

Figure 1. The conversion of CO_2 hydrogenation to formic acid via carboxylate (COOH) intermediate.

Keywords: CO_2 Hydrogenation, Pt-Boron nitride nanosheets, DFT.

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The theoretical study of catalytic CO_2 hydrogenation to formic acid over a metal-decorated carbon nanocone

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ABSTRACT

Carbon dioxide (CO_2), a greenhouse gas is one of the most prominent pollutant that must be resolved immediately. Among the CO_2 chemical conversion, Formic acid (FA) is the most interested product which will be used in many various applications. For the catalytic conversion of CO_2, Carbon nanocones (CNC) are one of the most interesting materials for CO_2 hydrogenation to FA. In this work, we addressed the potential catalytic role of metal-decorated defective carbon nanocones (M-dCNC) in CO_2 hydrogenation reaction to FA following equation; $CO_2 + H_2 \rightarrow HCOOH$, by density functional theory (DFT) calculations. We demonstrated that the combination of highly reactive metal atoms and defective CNC makes the M-dCNC a mono-dispersed atomic catalyst for CO_2 hydrogenation reaction. In term of various metals for CO_2 conversion reaction, our calculations showed that Pt-decorated defective carbon nanocone (Pt-dCNC) is the most suitable catalyst for the CO_2 hydrogenation to FA. Following the catalytic reaction pathway, the presence of hydrogen molecule (H_2) in the system plays a significant role in producing the FA on the Pt-dCNC catalyst by firstly dissociated H_2, then spilled-over H atom into the CNC surface. Moreover, we found that The Pt-formate species can be converted into formic acid via the heterolytic cleavage pathway with rate determining step of 16.31 kcal/mol.

Keywords: Density functional theory (DFT); CO_2 hydrogenation reaction; formic acid (FA); Carbon nanocone (CNC); Platinum (Pt)

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Ag_7Au_6 cluster as a highly active catalyst for CO oxidation: Theoretical study

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ABSTRACT

Using density-functional theory (DFT), we investigated the oxidation of CO on Ag_7Au_6 alloy metal nanocluster. The structures of intermediates and transition states on the potential-energy surfaces were located using the nudged-elastic-band (NEB) method. According to calculation results, the adsorption energies of the most stable configuration of CO, O_2 and CO_2 on the Ag_7Au_6 catalyst were used for CO oxidation mechanism. In addition, we also investigated reaction pathway for CO oxidation by O_2 on Ag_7Au_6 catalyst including stepwise adsorption and coadsorption mechanisms.Calculation results showed that, coadsorption mechanism with coupling of CO and O_2 molecules to form intermediate OCOO has the least energy barrier on the Ag_7Au_6 nanocluster, whereas the dissociation of the O–O bond of OCOO to form CO_2 and O on the Ag_7Au_6 nanocluster is the easiest process with a 0.10 eV barrier height. The coadsorption mechanism was found to be more thermodynamically and kinetically favorable, with the rate-determining activation barrier of 0.26 eV. Such a low activation barrier indicates that the Ag_7Au_6 catalyst is active for CO oxidation at room temperature and it could be a good candidate catalyst with lower and higher activity.

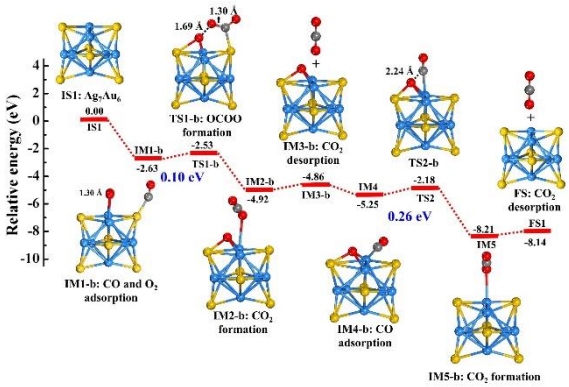

Figure 1. The calculated structures and the corresponding energy profile in following CO oxidation on Ag_7Au_6 cluster via coadsorption mechanism

Keywords: CO oxidation, Density Functional Theory, coadsorption mechanism, stepwise adsorption mechanism

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Molecular dynamics simulations of hyaluronic acid in water

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ABSTRACT

Hyaluronic acid (HA) is a linear polysaccharide with repeating disaccharide units, each of which is composed of glucuronic acid and N-acetyl glucosamine. HA is one of the major matrix substances in extracellular tissue of vertebrates. One of important properties of HA is high water affinity which makes it to become a moisturizer. Most of skin-care products have HA being a main ingredient. Many researches reported that low-molecular weight HA (LMW HA, MW < 50 kDa) have high permeability through skin. The aim of this work is to evaluate the effect of size of LMW HA on the hydration properties and their conformations by all-atom molecular dynamics (MD) simulations. Straight-chain structures of HA of various sizes including 5, 10, 20, 30, 40 and 50 units were constructed based on the conformational geometry of the crystal structure (PDB code 2BVK), and subsequently subjected for 50 ns MD simulations in the gas phase to examine conformational states at different chain lengths. MD results showed a decrease of radius of gyration (Rg) for all the HA models, suggesting folded structures of HA. 100 ns MD simulations of HA at 5 units in aqueous solution illustrates that its Rg value is not significantly decreased. The structure of the first hydration shell of HA extracted from the radial pair distribution functions (RDF) indicates that there are, on average, about 24 water molecules per disaccharide unit.

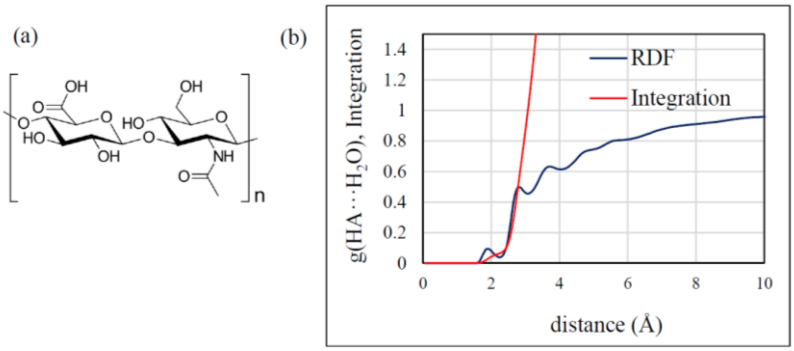

Figure 1. a) Monomer of HA (b) Normalized RDF between HA 5 units and water

Keywords: Hyaluronic acid, Molecular dynamics simulation, Conformations, Hydrations

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Computational Study of Binding Mode of Depsidones in Vascular Endothelial Growth Factor Receptor-2

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ABSTRACT

Colon cancer is one of the most common types of cancer and leading causes of death worldwide. There are a number of proteins involved in molecular pathway causing colon cancer. Vascular endothelial growth factor receptor-2 (VEGFR-2), a protein controlling the formation of new blood vessel, is an interesting protein target in colon cancer treatment. Depsidones are compounds containing two aromatic rings joined by an ester bond and an ether bond. They are found as secondary metabolite in lichens. In this research fourteen depsidones, isolated from the fungus Chaetomium brasiliense, were theoretical studied in order to know their binding affinity to VEGFR-2. All depsidones were optimized their geometry. The structures of two major forms of each depsidone were observed. Then, molecular docking between depsidones and VEGFR-2 were done by using GOLD. From the docking results, all depsidones showed similar binding mode except one depsidone – it also gave highest fitness score and formed strong hydrogen bond with Glu917, Phe918 and Cys919 amino acids.

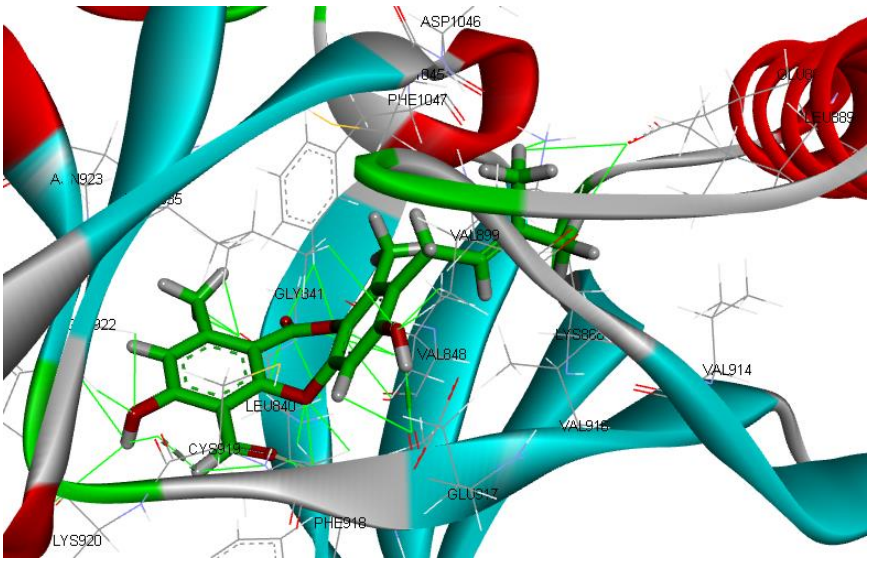

Figure 1. Binding mode of the depsidone with highest fitness score and VEGFR-2.

Keywords: Colon Cancer, Vascular Endothelial Growth Factor Receptor-2, Depsidone, Molecular Docking

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Delivery of Alpha-mangostin through biological membrane using cyclodextrins: A molecular dynamics simulation study

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ABSTRACT

Alpha-mangostin (MGS), a traditional Thai medicine, is commonly used to treat skin inflections, diarrhea, and chronic wounds [1]. Although MGS has interesting properties, its has low solubility and stability leading to limitations in its pharmaceutical applications. The complex formation with cyclodextrins (CDs) is well-known to enhance solubility and bioavaility properties of hydrophobic compound [2]. In this work, we aim to study the release process of MGS from CDs (i.e., βCD, 2,6-dimethyl-βCD (DMβCD) and 2-(2-hydroxypropyl)-cyclodextrin (HPβCD)) into the 1-dipalmitoyl-2-oleyl-*sn-glycero*-3-phosphatidylcholine (POPC) based on molecular dynamics (MD) simulation. From over a few hundred nanoseconds, all inclusion complexes can adsorb on POPC membrane and MGS/DMβCD complex somewhat insert through membrane surface and interact with the polar head groups via hydrogen bond formation. However, the MGS cannot spontaneously release from hydrophobic cavity of CDs and penetrate into the lipid bilayer membrane. This is therefore MD simulation in a couple with umbrella sampling method was further applied on the system to investigate the delivery of MGS through lipid bilayer. The release process from different CDs was discussed and compared.

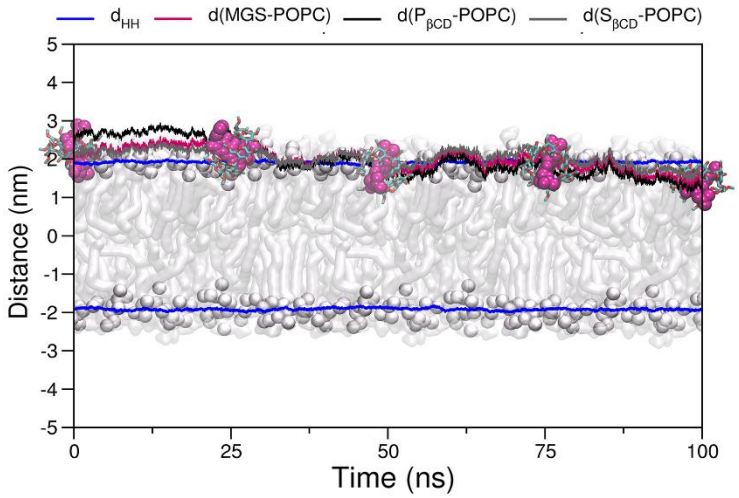

Figure 1. Dynamics of MGS/DM□CD inclusion complex into POPC lipid bilayer.

Keywords: Alpha-magostin, cyclodextrin, biological membrane, permeability, molecular dynamics simulation

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Efficient Two-dimensional Ion Pairing Free Energy Surface Computation with Gaussian Process Regression

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ABSTRACT

Free energy computation is an important tool in chemistry of aqueous solutions, providing a glimpse into the dynamical properties of both the solvent and the solutes through the minimum free energy pathway (MFP). However, capturing both the solvent and the solutes' dynamics requires more than one collective variables (CV), making multidimensional free energy computation along the dimensions of all CVs a costly undertaking with traditional methods. In this work, we computed the two-dimensional free energy landscapes of LiCl and NaCl in aqueous solutions to study the mechanistic picture of the transition between the solvent-separated ion pair (SSIP) and the contacted ion pair (CIP) configurations. We employed both the solvent and the solute variables using a combination of well-tempered metadynamics (WT-MTD) and Gaussian process regression (GPR), which is the first application of such method in a multidimensional case beyond model systems. We found that the error of the two-dimensional surfaces computed relative to reference surfaces obtained from umbrella sampling (US) is in the order of 0.1 kcal/mol, which is small compared to the CIP – SSIP barrier heights, which can be achieved using far less total simulation efforts relative to similar works in the past. The MFPs of both systems suggest that the transition from SSIP to CIP is through the dissociative mechanism, where the cation loses one water of its first solvation shell in order to accommodate the anion in the CIP form. Our overall results also suggest that, in accordance with the previous introduction of this scheme, the combination of WT-MTD and GPR offers a large efficiency gain even in the one-dimensional case for an acceptable error, which paves the way for further applications in multidimensional free energy computations for computationally expensive chemical simulations.

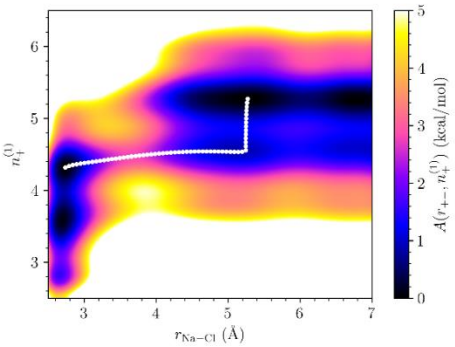

Figure 1. A two-dimensional free energy landscape of NaCl in aqueous solution using the interionic distance (r_NaCl) and the modified number of water molecules in the cation's first solvation shell (n_+^((1))) as the collective variables, with MFP computed by Zero-temperature String Method (ZTS).

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Computational Modeling of Cationic Metallocene Polymerizations of 2-Oxazoline

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ABSTRACT

Poly(2-oxazolines) are biocompatible and nontoxic materials that are attracting attention in industrial and biomedical applications. These polymers were typically obtained by cationic ring-opening polymerization (CROP) of 2-R-oxazoline monomer, in which their properties can be tuned by its R group. Here we have conducted a density functional theory study on the CROP reaction with 2-methyl- and 2-phenyl-oxazoline monomers using cationic complex [Cp2ZrMe]+[B(C6F5)4]- as catalyst systems. In this talk, we will focus on three elementary steps of the CROP process including ion-pair formation and dissociation, initiation and first propagation. In addition, the effects of the R group, cocatalyst and solvent on the polymerization activity have also been studied. These results provide important information that can be used to rationalize several previous experimental observations.

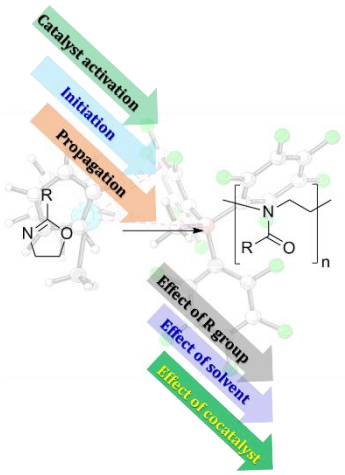

Figure 1. The cationic polymerization of 2-methyl and 2-phenyl oxazoline by a zirconocene/borate catalyst

Keywords: Polyoxazoline, cationic polymerization, metallocene, boron activator, DFT

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The reaction between Criegee intermediates and sulfur dioxide: not really barrierless

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ABSTRACT

Criegee intermediates have gained great attention for its important roles in atmospheric chemistry; one potential role is the oxidation of SO_2 in the atmosphere. The reaction rate coefficients between Criegee intermediates and SO_2 are reported[1-7] in the range of 2×10^{-11} to 2×10^{-10},cm^3 s^{-1}, which are very fast and always considered as barrierless reactions. However, after careful study on these reactions, we found that for most Criegee intermediates, there is a transition state in the process of reaction and the barrierless assumption may not be valid.

Keywords: Criegee intermediate, *ab initio* calculation, barrierless reaction, transition state.

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Dynamics Simulation of Excited-State Intramolecular Proton Transfer Reactions of 2,5-bis(2'-benzoxazolyl)hydroquinone

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ABSTRACT

The dynamics simulations of the excited-state intramolecular proton transfer (ESIPT) of 2,5-bis(2'-benzoxazolyl)hydroquinone (BBHQ, Figure 1) have been performed on their lowest energy structures using time-dependent density functional theory (TDDFT) at TD-B3LYP/SVP level. Our dynamics simulations showed that there are two possible mechanisms of the ESIPT processes: a) single proton transfer and b) double proton transfer. The ESIPT mechanism of isolated BBHQ elucidates that single proton transfer is more likely to take place in comparison with the double proton transfer reaction. However, water might help double proton transfer to occur by stabilizing keto tautomer after proton transfer completed.

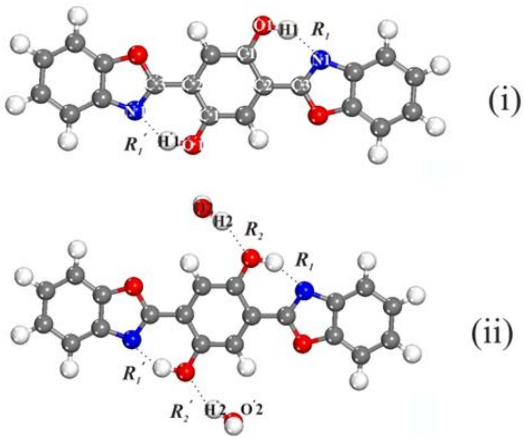

Figure 1. Optimized geometries of 2,5-bis(2'-benzoxazolyl) hydroquinone (BBHQ) computed by B3LYP/SVP level. (i) Isolated BBHQ and (ii) BBHQ with water molecules.

Keywords: ESIPT, Dynamics simulation, 2,5-bis(2'-benzoxazolyl)hydroquinone.

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Theoretical investigation of Propane Dehydrogenation on Ni(111) surface

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ABSTRACT

Propane dehydrogenation (PDH) on Ni(111) surface to give propylene and side reactions of cracking and deep dehydrogenation have been theoretically investigated by density functional theory (DFT) calculation. The adsorption of propane on Ni(111) surface is physisorption whereas that of propylene is chemisorption. Charge difference along with Bader charge analysis depict the charge movement from Ni(111) surface to adsorbed molecules (propane and propylene). The PDH reaction can occur in two dehydrogenation steps. The first step is dehydrogenation to convert propane to form propyl. Then, the second step is conversion of propyl to form propylene on Ni(111) surface. The first step of PDH reaction occurs in two different pathways: 1-propyl as pathway A and 2-propyl as pathway B. The dehydrogenation of propane to form 1-propyl in pathway A is more feasible than that of 2-propyl because of more kinetic favorable of PDH reaction and more thermodynamic stable of 1-proply on Ni(111) surface. The side reactions of C-C bond cracking and deep dehydrogenation are also considered comparing with PDH process to describe the selectivity of propylene production. The C-C bond cracking along PDH process is more difficult to take place than dehydrogenation reaction supported by higher energy barrier of cracking process. After PDH process, the high desorption barrier of propylene limits propylene production from Ni(111) surface leading to unwanted reaction of propylene cracking and deep dehydrogenation causing the low selectivity of propylene production. Understanding of the reaction mechanisms of PDH and side reactions on Ni(111) surface is useful for designing and developing the better selective Ni catalyst by increasing the reactivity of propylene desorption and inhibiting the side reaction of C-C bond cracking and deep dehydrogenation.

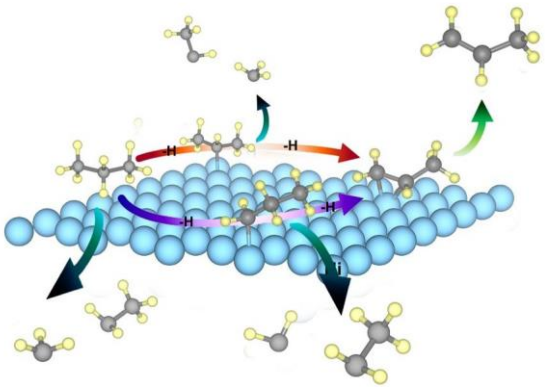

Figure 1. The possible mechanisms of PDH and side reactions on catalyst surface

Keywords: Propane dehydrogenation, Deep dehydrogeantion. C-C bond cracking, DFT

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Replica Exchange Molecular Dynamics Simulations of 2-Hydroxypropyl-β-Cyclodextrin

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ABSTRACT

2-Hydroxypropyl-β-cyclodextrin (HPβCD) has the unique properties to enhance stability and solubility of low water-soluble compounds. Understanding structural properties of HPβCD based on the number of substituted 2-hydroxypropyl (HP) is critical for molecular encapsulation. In this work, replica exchange molecular dynamics (REMD) simulations were performed to investigate conformation of single- and double-sided HP-substitution called as 6-HPβCDs (1) and 2,6-HPβCDs (2), respectively. Conformational analyses such as structural distortion, radius of gyration, circularity and cavity self-closure of the HPβCDs were performed. The results demonstrate that glucose subunits in both 6-HPβCDs and 2,6-HPβCDs have lower chance to flip than in βCD. Moreover, HP groups occasionally block the hydrophobic cavity of HPβCDs, thus hindering the drug inclusibility. Moreover, the cavities of HPβCDs with high number of HP substitutions are more likely to be blocked. Overall, 6-HPβCDs with three and four HP substitutions are highlighted as the most suitable structure for guest encapsulation.

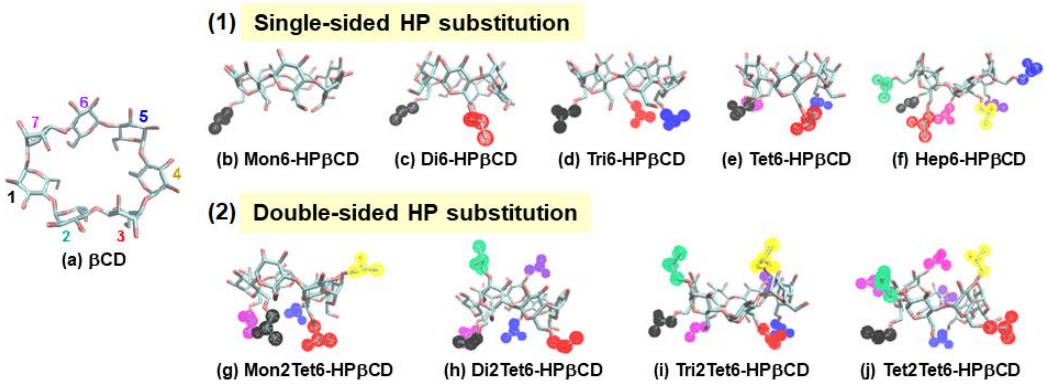

Figure 1. The HPβCD model of single- and double-sided HP-substitution called as 6-HPβCDs (1) and 2,6-HPβCDs (2), respectively.

Keywords: 2-Hydroxypropyl-*β-cyclodextrin* (HP*β*CD); Replica exchange molecular dynamics (REMD); Cavity self-closure

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The pH-Dependent Shaping of Water-filled Crevice in the Hv1 Channel

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ABSTRACT

The voltage-gated proton-selective (Hv1) channel plays a critical role in various physiological processes by proton extrusion. The pH-sensing mechanism of the Hv1 channel should promote a structural transition according to the previous reports.[1] A voltage-sensing domain (VSD) of the Hv1 channel which is responsible for a proton pore might undergo conformational change at different pH. In this study, molecular dynamics (MD) simulation was used to elucidate the influence of pH condition on the Hv1 structure. The resting state of a recently determined X-ray crystal structure of a chimera of mouse Hv1 channel (mHv1cc) was used. The transmembrane (TM) segments of the VSD significantly exhibit a pH-dependent conformational change (Figure 1). Modification of the protonation states of highly conserved charged residues through the VSD region induces the structural change of TM segments as shown in Figure 1. Rearrangement of a hydrogen-bond network was observed. At acidic pH, packing of the VSD core becomes loose resulting in a larger pore size (Figure 1). This affects a shaping of water-filled crevice and packing of the hydrophobic layers. Furthermore, a bipolar orientation of water molecules with dipole inversion was observed. The results also provide the evidence on tuning water orientation by the charged residues under different pH values.

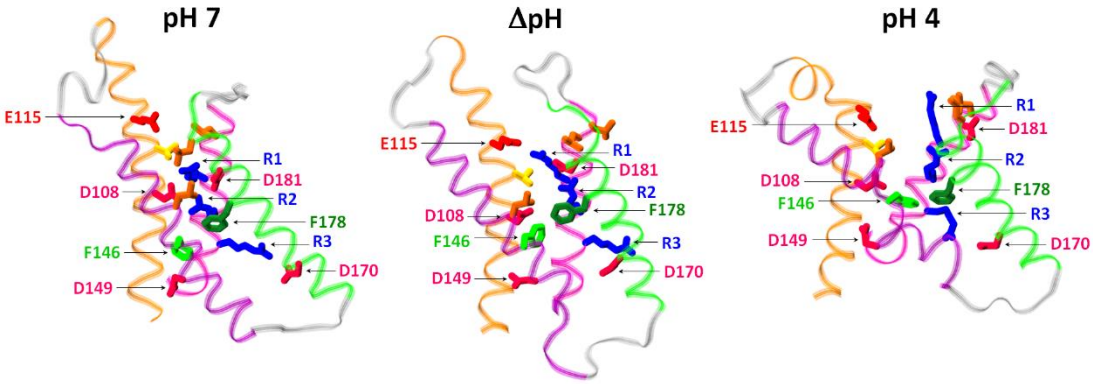

Figure 1. Conformations of the VSD region at various pH conditions. The TM segments and focusing residues are shown in helix and licorice styles with different colors, respectively.

Keywords: MD simulation, Hv1 channel, pH dependence.

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Electronic and photophysical properties of derivatives of 2-phenylbenzothiazole and 2-(2´-hydroxyphenyl) benzothiazole: Effect of intramolecular hydrogen bonding

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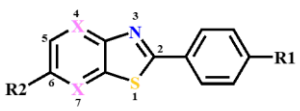
ABSTRACT

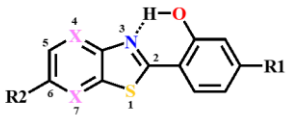
Photophysical properties of 2-phenylbenzothiazole (PBT) denoted as a No-PT type compound and 2-(2´-hydroxyphenyl)benzothiazole (HBT) denoted as a PT type compound as well as their derivatives have been investigated using six different DFT and TD-DFT methods. The B3LYP exchange-correlation functional with 20% HF exchange is found to be the most suitable method for reproducing experimentally photophysical data. Overall, the simulated absorption and emission spectra of all derivatives are red-shifted compared with their parent compounds, PBT and HBT, except emission spectrum of TPy-1 is blue-shifted. Especially, TPy-3 and HTP-2, of which the carbon atoms at 4,7-positions of the benzothiazole core are replaced by nitrogen atoms and hydrogen atoms in the 2,6-positions are substituted by dimethylamino phenyl groups, show more red-shifted absorption spectra than other compounds caused by lone pair electron of nitrogen atoms and electron donating group that has the effect on the π-conjugated system. In addition, TPy-4 and HTP-3 also have the similar effect on π-conjugated system. As expected, the calculated Stokes shifts of the PT type compounds are larger than that of the No-PT type compounds, because of the tautomer formation through the excited state intramolecular proton transfer (ESIPT) process. The potential energy curves (PECs) scanned along the proton transfer (PT) coordinate of the PT type compounds reveal that the ESIPT process is more likely to proceed in the S_1 state. The ESIPT process in HBT, HTP and HTP-1 occurs with a small barrier or barrierless, whereas that in HTP-2 and HTP-3 involves a higher barrier. The PT barriers were found to be in the order of HTP ~ HBT > HTP-1 > HTP-2 > HTP-3. The knowledge accumulated through these studies is expected to be useful for the rational design of fluorescent molecular probes.

No-PT type



Structure	X	R_1	R_2
PBT	C	H	H
TPy-1	N	H	H
TPy-2	N	H	Ph
TPy-3	N	$N(CH_3)_2$	Ph-$N(CH_3)_2$
TPy-4	N	OCH_3	Ph-OCH_3

PT type



Structure	X	R_1	R_2
HBT	C	H	H
HTP	N	H	H
HTP-1	N	H	Ph
HTP-2	N	$N(CH_3)_2$	Ph-$N(CH_3)_2$
HTP-3	N	OCH_3	Ph-OCH_3

Figure 1. Molecular structures of all compounds PBT and its derivatives (No-PT type) and HBT and its derivatives (PT type)**Keywords:** MD simulation, Hv1 channel, pH dependence.

Keywords: 2-Phenylbenzothiazole derivatives, 2-(2'-hydroxyphenyl)benzothiazole derivatives, TD-DFT, ESIPT

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Heteroatom effect on electronic and photophysical properties of 3-hydroxyquinolin-4(H)-one and its derivatives enhancing in the excited-state intramolecular proton transfer processes: A TD-DFT study on substitution effect

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ABSTRACT

The effect of hetero oxygen and nitrogen substituted of 3HX derivatives (3HQ, 3HF, 3HTF, and 3HSO where X=NH, O, S, and SO_2 respectively) on the electronic, photophysical properties, and excited-state intramolecular proton transfer (ESIPT) was investigated using density functional theory (DFT) and time-dependent DFT (TD-DFT). Geometries and absorption spectra as well as emission spectra of 3HX derivatives were carried out by using DFT and TD-DFT at the B3LYP/TZVP level. The important parameters for bond distances involving the intramolecular H-bond reveal that H-bonds of 3HX derivatives in excited-state are stronger than those in the ground state, supported by the red-shift of O–H vibrational modes in the excited-state. The heteroatom substitution of 3HX causes the red-shift emission spectra, implying that the lone pair of electron in the substituted heteroatom has the effect on the intramolecular charge transfer. In addition, results of frontier molecular orbitals show that vertical $S_0 \rightarrow S_1$ transition of these molecules corresponds essentially to the excitation from HOMO (π) to LUMO (π*). The potential energy curves (PECs) of intramolecular proton transfer (IntraPT) process of all derivatives were used to investigate the occurrence of ESIPT. The hetero sulfur on X positions of 3HX derivatives could easily facilitate the ESIPT process because sulfur makes O1–H1 bond of 3HTF weaker than those of other derivatives confirmed by its more red-shifted vibrational modes in the excited-state compared with other heteroatom substitutions, resulting in lower ESIntraPT barrier. The obtained information of the electronic structure, the photophysical property and the chance of ESIPT of heteroatom substituted 3HX molecules are useful for the molecular design of fluorescent molecular probes.

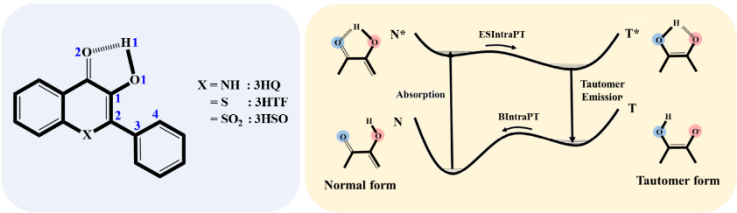

Figure 1. Schematic of 3HQ, 3HF, 3HTF, and 3HSO and Schematic diagram of the general ESIPT process, a proton donor and proton acceptor are circled with red and blue, respectively.

Keywords: Excited state proton transfer (ESPT), 3-Hydroxyquinolin-4(H)-one, Heteroatom effect, B3LYP

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Density functional theory insight towards the design of ionic liquids for CO_2 capture

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ABSTRACT

A systematic density functional theory (DFT) has been employed to obtain information at the molecular level on the key parameters related to efficient CO_2 absorption by ionic liquids (ILs). A set of 50 ILs, for which high thermal stability is expected, has been selected. CO_2 absorption over ILs was predicted based on the various DFT functional and basis sets without prior experimental knowledge of the compounds' features. Then, interactions between CO_2 and ILs were analyzed through HOMO-LUMO energy gap, charge transfer and effects of additional functional groups. This work provides valuable information about important factors at the molecular scale to obtain the rational design of high CO_2 absorption in ILs, which is necessary for further implementation of task-specific ILs in the future.

Keywords: CO_2 absorption, Ionic liquid, DFT.

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Path Integral Molecular Dynamics Simulations for Muoniated Thioformaldehyde Radicals

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ABSTRACT

A considerable amount of knowledge for muonium (Mu; complex of a positive muon (μ+) atom and an electron) chemistry has been accumulated for over 30 years1. A muon has a smaller mass and larger magnetic moment than those of proton. Because of these unique features, Mu atom is used as the muon spin resonance/rotation/relaxation (μSR), where hyperfine coupling constant (HFCC) is a good index for the magnetic interaction between electron and muon spins. In this study, we investigated the structures and "reduced" HFCC values for muoniated and hydrogenated thioformaldehyde radicals, a Mu or H atom is added to carbon atom (C adduct) or sulfur atom (S adduct) of the thioformaldehyde compound (H2C=S) using the on-the-fly ab initio path integral molecular dynamics (PIMD) method2, 3, which can include both nuclear quantum and thermal effects. The single point energy of C adduct structure with CCSD/aug-cc-pVDZ (optimized with MP2/6-311++G(d,p)) level is 13.48 lower than that of S adduct structure, corresponding the previous study4. The HFCC values from a simple geometry optimization calculation of C adduct and S adduct are 22.42 and -7.39 MHz, respectively, at the BHandHLYP/6-31+G(d,p) level. In the case of C-adduct, the reduce HFCC values of the muoniated thioformaldehyde radical by our PIMD simulation is slightly larger than that of hydrogenated radical with the same calculation level. We found that the local molecular structures affect the HFCC values, particularly, the Mu——C bondlength in the muoniated thioformaldehyde radical is lengthen due to the large nuclear quantum effect of moun.

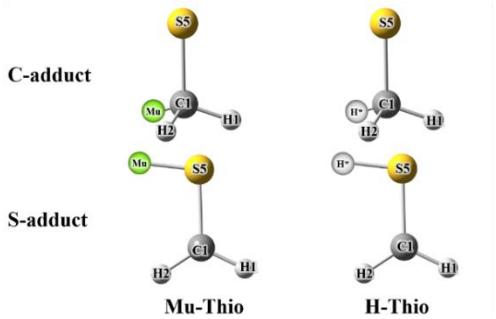

Figure 1. The optimized structure of muoniated and hydrogenated thioformaldehyde radicals (Mu-Thio and H-Thio).

Keywords: Muons, Thioformaldehyde, Hyperfine structure, PIMD simulations, Nuclear quantum effect.

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Inhibitory of Influenza H1N1 Hemagglutinin with Flavonoid Compounds from Thai Herbs

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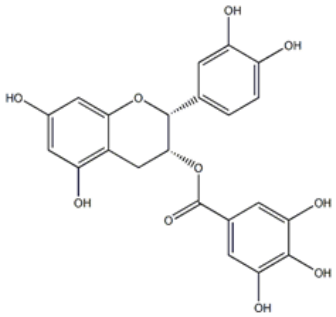
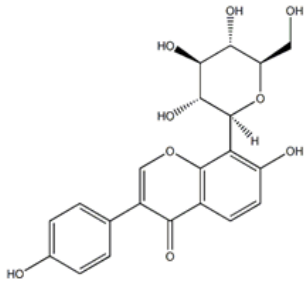
ABSTRACT

Outbreaks of H1N1 influenza are a serious concern for public health. In the reproductive cycle of the influenza virus, hemagglutinin (HA) is the primary protein responsible for binding to glycan receptor sites on the host cell surface. The molecular docking of human H1 HA complexed with 30 flavonoid compounds from Thai herbs were performed to screen the lead compounds on the criteria of binding free energy, hydrogen bond formation with key residues of HA. The docking results showed that epicatechin gallate (13) and puerarin (27) have high binding energy to HA, which the binding energies of -7.2 and -7.89 kcal/mol, respectively. Then, the molecular dynamic simulation (MD) of 13-HA and 27-HA complexes were performed to study the role of HA key residue, structural behavior, hydrogen bond formation and binding free energy. All calculations of the both complexes were carried out using the AMBER 14 software package. The MD simulations were carried out for 70 ns where the production phase started from 31 ns to 70 ns. From the results, it can be suggested that epicatechin gallate (13) and puerarin (27) are a good opportunity for drug developing toward influenza H1N1 hemagglutinin.



epicatechin gallate (13)



puerarin (27)

Keywords: Hemagglutinin; Flavonoid; Molecular Docking; Molecular dynamics simulation

An ONIOM study on the 7-hydroxyl-4-methylcoumarin synthesis with H-Beta zeolite

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ABSTRACT

In this study, the synthesis of 7-hydroxyl-4-methylcoumarin via the Pechmann condensation reaction catalyzed by H-Beta zeolite catalysts has been examined by ONIOM approach. Adsorptions and reactions taking place inside the 5T:34T (T means tetrahedral of Si or Al atoms) of H-Beta zeolite were calculated with ONIOM(MP2:M06-2X). The total activation energies for the transesterification, the intramolecular hydoxylalkylation and the dehydration were calculated to be 13.6, 2.8 and 17.9 kcal mol-1, respectively. This study provides detailed understanding for the Pechmann condensation reaction with the zeolite catalyst.

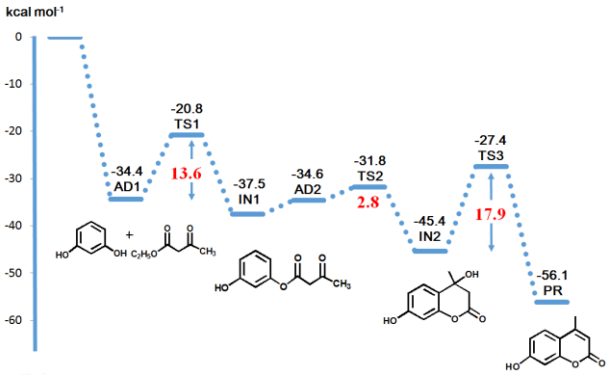

Figure 1. Reaction Pathway of Pechmann reaction for the 7-hydroxyl-4-methylcoumarin synthesize with H-Beta zeolite model 5T:34T at the ONIOM(MP2:M06-2X) approach. The relative energies are in kcal mol^{-1}.

Keywords: Pechmann reaction, coumarin synthesis, ONIOM.

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Effect of Impurities in $MgCl_2$ Support for Polymerization of Ethylene with Heterogeneous Ziegler-Natta Catalyst: A DFT Study

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ABSTRACT

The $MgCl_2$-supported Zingler-Natta (ZN) catalyst is a very important complex for polymerization of olefins. Previous experimental studies have shown that doping inorganic salts can change the distribution of defects of the $MgCl_2$ support and can enhance the catalytic performance of the ZN active site. Although great progress has been made in fundamental investigations on catalyst structure and the polymerization mechanism, many important question regarding the relationships between the microstructure of the active species and their catalytic performance, the role of doping agent on the electronic properties of the ZN active centers remain the subjects of debates. We have used the unrestricted M06-L with a combination of 6-31G(d,p) basis set for non-metal atoms + LANL2DZ ECP for metal atoms to demonstrate the role of impurity on the activity of the Ti active center. The electronic ground state of Ti(R)/Mg_2**X**Cl_3 systems is singlet (**X** = Mg(II), singlet (**X** = Zn(II), and quintet (**X** = Fe(II) spin states, respectively. Initial coordination of the C_2H_4 molecule to Ti(C_2H_5)/Mg_2**X**Cl_3(**X** = Mg(II), Zn(II), and Fe(II)) proceed smoothly to give Ti(C_4H_9)/Mg_2**X**Cl_3(**X** = Mg(II), Zn(II), and Fe(II)) intermediate. The activation energy of the first insertion is 4.8, 3.7, and 5.4 kcal/mol for the undoped, Zn-doped, and Fe-doped systems, respectively. However, the reaction rate constant of the first insertion over the undoped system is equal to the rate constant of the first insertion over the Fe-doped system and significantly higher than the Zn-doped systems due mainly to the entropic effect. For the second propagation, the subsequent formation of the Ti(C_6H_{13})/Mg_2**X**Cl_3(**X**= Zn(II) and Fe(II)) has an activation energy slightly lower than that of the reaction over the undoped system (E_a = 3.0, 3.0, and 5.4 kcal/mol for the Zn-doped, Fe-doped, and undoped systems, respectively). For the third propagation, the activation energy of the formation of Ti(C_8H_{17})/Mg_2**X**Cl_3(**X**= Zn(II) and Fe(II)) is lower than that of the reaction over the undoped system(E_a = 3.5, 4.1 and 4.4 kcal/mol for the Zn-doped, Fe-doped, and undoped systems, respectively). The calculated activation energies of the chain propagation reaction over the undoped system agree well with the experimental data from Barabonov *et. al.* (4 kcal/mol). Interestingly, impurities in the $MgCl_2$ slightly weaken the adsorption energy of ethylene molecule. As a result, the reduction of heat of adsorption of the reactant leads to the lowering of the apparent activation energy of chain propagation. Therefore, the impurity in the support can greatly promote the reactivity and catalytic activity of the $MgCl_2$-supported Zingler-Natta (ZN) catalyst.

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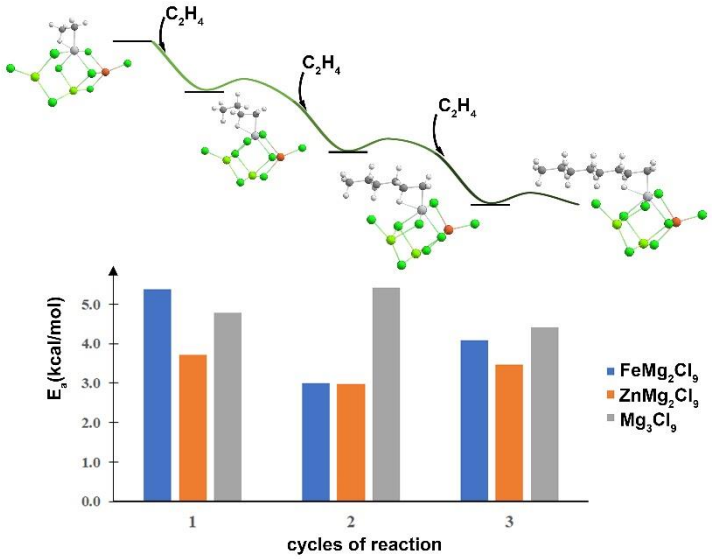

Figure 1. Activation energies for three cycles of C_2H_4 polymerization catalyzed by $Ti(C_2H_5)/Mg_2\mathbf{X}Cl_3$(**X** = Mg(II), Zn(II), and Fe(II)) catalysts.

Keywords: DFT calculations, Ziegler-Natta catalyst, Ethylene polymerization

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Computational calculation of CO_2 adsorption in MIL-127(Fe) Metal Organic Framework

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ABSTRACT

The Metal Organic Frameworks (MOFs) or Porous Coordination Polymers (PCPs) have been reported to be powerful materials for their usability and applications. The components of this porous solid materials are metal cluster connected with the organic molecules. Material of Institute Lavoisier-127 (MIL-127) being a subclass of MOFs can be used for gas separation, gas storage, catalysis, and drug encapsulation. In this work, we would like to gain insight into the adsorption and diffusion behavior of carbon dioxide in MIL-127 using Gibbs Ensemble Monte Carlo (GEMC) and Molecular Dynamics (MD) simulations. Firstly, the calculated adsorption isotherm was compared with the experimental result [1] to find the most suitable force field parameters. The radial distribution function, probability density distribution, and site of the lowest potential energy were calculated in order to understand behavior of carbon dioxide in MIL-127. Finally, selected parameters were used to investigate the structure and self-diffusion of the guest molecules in the MIL-127.

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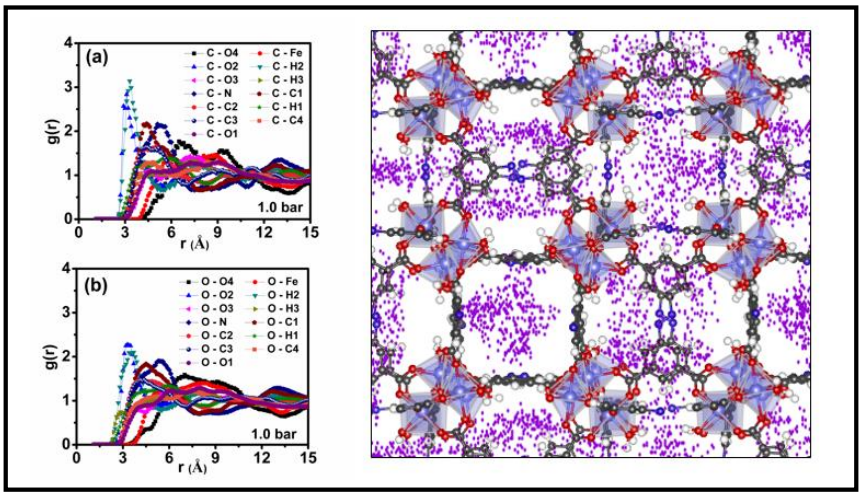

Figure 1. Radial Distribution Functions and Probability density of CO_2 in Material of Institute Lavoisier-127 (MIL-127)

Keywords: Computational calculations, Metal Organic Framework, Adsorption, Diffusion

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ELECTRONIC PROPERTIES OF PYRENE ADSORBED ON GRAPHENE NANOFLAKES

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ABSTRACT

Graphene has good conductivities, good thermal properties, extremely high surface area, light weight, etc. Therefore, it graphene has been a subject for large numbers of researches. We have particularly interest in the electronic properties of graphene nanoflakes, which is the finite size graphene. Junghyun Lee et al [1] suggested that electronic properties of graphene can be modified by noncovalent interactions with aromatic molecules through π-π interaction such as pyrene. In this work, we studied effect of substituents of π-conjugated compounds on adsorption energy and electronic properties with GNF, two different GNF models, hexagonal graphene nanoflake (HGN) and rhomboidal graphene nanoflakes (RGN) were studied as shown in Figure 1. Pyrene derivatives with either electron-withdrawing substituents such as 1-nitropyrene (Py-NO_2) 1-pyrenesulfonic acid (Py-SO_3H), 1-pyrenecarboxylic acid (Py-CO_2H), and donating substituents such as 1-aminopyrene (Py-NH_2), 1-hydroxypyrene (Py-OH), 1-methylpyrene (Py-CH_3) as adsorbates were considered. The calculations were performed density functional theory method with PBE and M06-2X functionals and 6-31g basis set. Pyrene and all pyrene derivatives show strong adsorption with energy ranging from 18 to 20 kcal/mol. A slight shift in HOMO and LUMO was observed for RGN, while a more significant shift is noticed for HGN doped with $PyNH_2$ (0.74 eV). HGN doped with 1-nitropyrene ($PyNO_2$) provides the negative shift on LUMO (-0.44 eV). Therefore, HGN-PyNH2 and HGN-$PyNO^2$ can be made into a diode.

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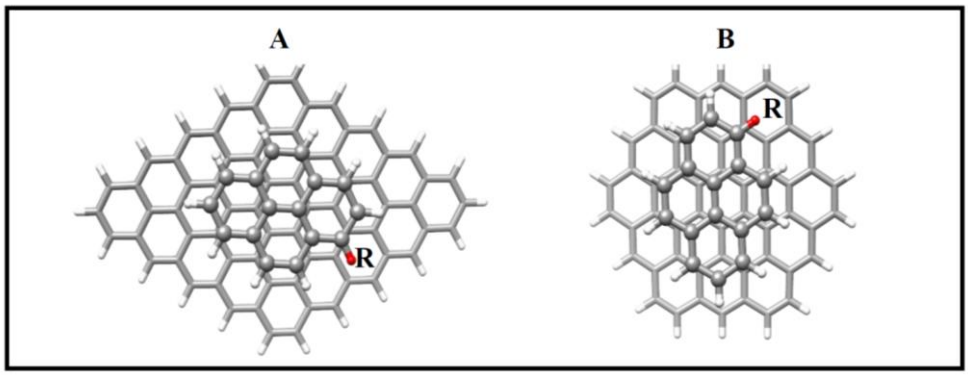

Figure 1. Schematic representation of RGN (A) and HGN (B) doped pyrene derivatives

R = CH3, OH, NH2 : electron donating groups

COOH, SO3H, NO2 : electron withdrawing groups.

Keywords: graphene nanoflakes, noncovalent interactions, pyrene

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Cooperation of Single Co Atom with Defect MoS_2 as a High Efficient Catalyst for HDO Reaction: A DFT Study

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ABSTRACT

The decoration of a single Co atom on a MoS_2 basal plane shows high-stability, -catalytic reactivity and -efficiency for the hydrodeoxygenation (HDO) reaction.[1] In this work, the roles of the single Co atom and sulfur defect for the deoxygenation of 4-methyphenol (4MP) toward toluene were investigated using density functional theory (DFT) calculation. The insights into the reaction mechanism of HDO and hydrogen activation were systematically determined on this catalyst. The DFT results show that the strong interaction of Co substituted sulfur vacancy on MoS_2 basal plane is responsible for the durability of the catalyst. The strongest 4MP and H_2 adsorption sites can be observed at the Co site. This Co site also plays an important role for the hydrogen activation process before one dissociated H is trapped at the nearby vacancy site. The most favorable pathway reveals that 4MP initially adsorbs on the Co atom with its carbon backbone followed by the C--OH bond dissociation. The dissociated hydroxyl moiety is bound to the pre-adsorbed H atom to form H_2O molecule, while toluene is formed and stabilized on Co atom. Our results demonstrate that both S vacancy and single Co sites are essential keys for enhancing the catalytic performance of monolayer MoS_2 catalyst for the HDO reaction.

Keywords: HDO, toluene, deoxygenation, MoS_2 catalysts, Co doped, DFT.

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Molecular Dynamics Simulation of Nanodiscs using Coarse-Grained model

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ABSTRACT

Membrane proteins are difficult to handle because of poor water solubility [1]. There are more limitations of the study than those of soluble proteins. One approach to solve this problem is to encapsulate the membrane protein with a nanodisc [2]. The nanodisc is a lipoprotein, which consists of a phospholipid bilayer that is surrounded by two polypeptide chains. The use of nanodiscs to encapsulate membrane proteins are of recent interest. However, there is little understanding of the physical properties at the molecular level. This study uses coarse-grained molecular dynamics (CG-MD) simulation [3] to investigate structure. dynamics and physical properties of nanodiscs in solution. This study has constructed two nanodisc model systems that have two different phospholipids: 1,2-Dimyristoyl-sn-glycero-3-phosphocholine (DPPC) and 2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine (POPC), which are encircled by apolipoprotein A-1. To study the influence of temperature on the stability and structural changes of the nanodiscs, the CG-MD simulations were performed at temperatures of 200, 300 and 400 K for a period of 1 microsecond. The results of each trajectory at each temperature, including root-mean-square deviation (RMSD), radius of gyration (Rg) and solvent accessible surface area show that the temperature affects both the structure and dynamics of the two nanodiscs. The nanodiscs have increased flexibility when temperature increases. Due to the increase in temperature, the interactions between proteins and phospholipids in the nanodiscs are weakened. As a result, apolipoprotein A-1 has loosely bound to the phospholipid. The protein and phospholipid molecules in the nanodiscs are loosely packed. This may reduce the stability of the nanodisc structure. Comparing the results between DPPC-nanodisc and POPC-nanodisc, it was found that the effect of temperature-induced structural change for DPPC-nanodisc is not as severe as POPC-nanodisc. For DPPC-nanodisc, changes in structural properties have the same direction as increases in temperature whereas changes in structural properties of POPC-nanodisc are uncertain as temperature increases. It seems that thermal response of POPC-nanodisc makes the structure to be less stable than DPPC-nanodisc.

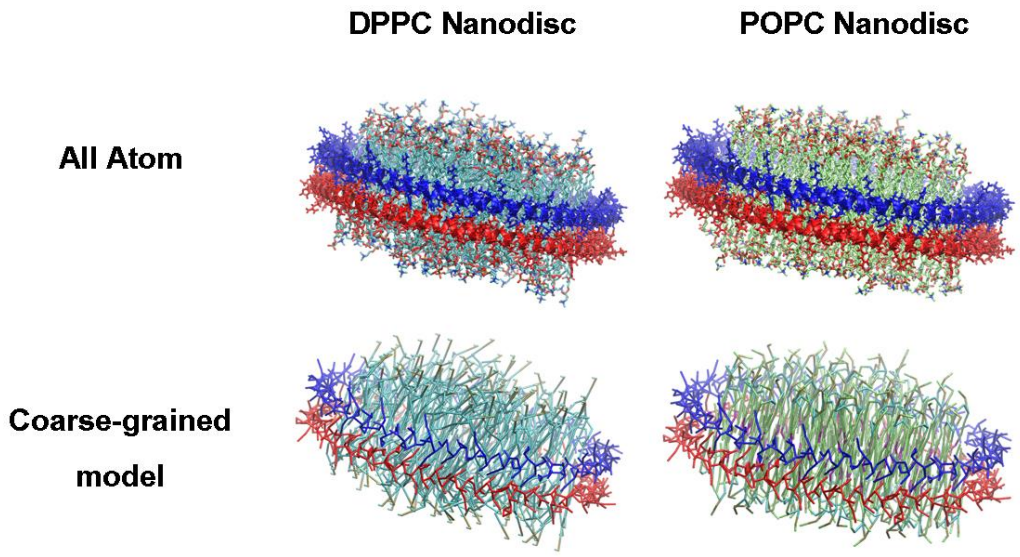

Figure. DPPC and POPC membrane model of nanodiscs in all-atom and coarse-grained

Keywords: Nanodisc, Coarse-Grained model, Molecular Dynamics simulation

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Computational Insight into Noncovalent Interaction of Solid Polymer Electrolytes on Graphene Surface for Fabrication of Supercapacitor Electrodes

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ABSTRACT

Solid electrolytes in electrochemical device have several advantages: no leakage, low flammability and high thermal stability with good processability. Polymeric electrolytes, which are poly(vinyl alcohol), poly(propylene carbonate), and i-carrageenan, were modelled on pristine graphene the electrode material for supercapacitors. Interfacial stability of complex models were computed using the third order self-consistent-charge density-functional tight-binding (DFTB3) with Grimme's dispersion correction. The results show that i-carrageenan has the strongest interaction with pristine graphene. This noncovalent interaction can be enhanced by using different types of nitrogen-doped graphene. Therefore, i-carrageenan with nitrogen-doped graphene could potentially be used for improving cycling ability of a fabricated supercapacitor.

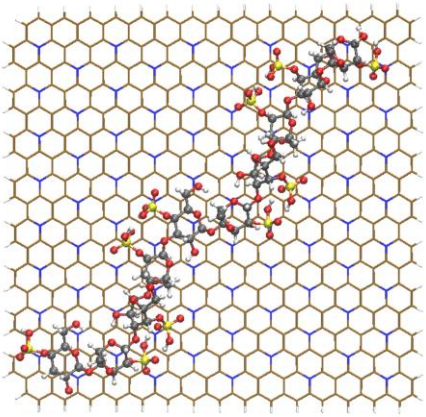

Figure 1. The optimized geometry of i-carrageenan on graphitic nitrogen-doped graphene.

Keywords: Graphene, Electrolytes, Supercapacitor, DFTB3, Noncovalent interaction energy.

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Lewis Acid Beta Zeolite Catalyzing the Catalytic Hydrogen Transfer of Furfural to Furfuryl alcohol: Insight from DFT Calculations

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ABSTRACT

Density Functional Theory (DFT) with M06-L functional have been performed to investigate the catalytic hydrogen transfer of furfural to furfuryl alcohol on cation exchanged Lewis acid BEA zeolite. The reaction mechanism commences with the dissociation of O-H bond of *i*-propanol to form propoxide intermediate. The hydrogen is then transferred from intermediate to the furfural methyl carbon to become furylmethoxy intermediate. The product of furfuryl alcohol is finally produced via proton abstraction from this intermediate. The hydrogen transfer step is rate-determining with the activation energies of 23.8, 28.3 and 31.2 kcal/mol for Li-SnBEA, Na-SnBEA and K-SnBEA, respectively. Therefore, the catalytic activity of Li-Sn-BEA zeolite should succeed over Na-Sn-BEA and K-Sn-BEA. The catalytic activity of different tetravalent metal centers (Sn, Zr and Hf) substituted Li-BEA zeolites is also considered. It is found to be in the order of Zr ≥ Hf > Sn. We also provide useful chemical descriptors to predict the hydrogen transfer step to be used to rapidly screen promising catalysts for this reaction.

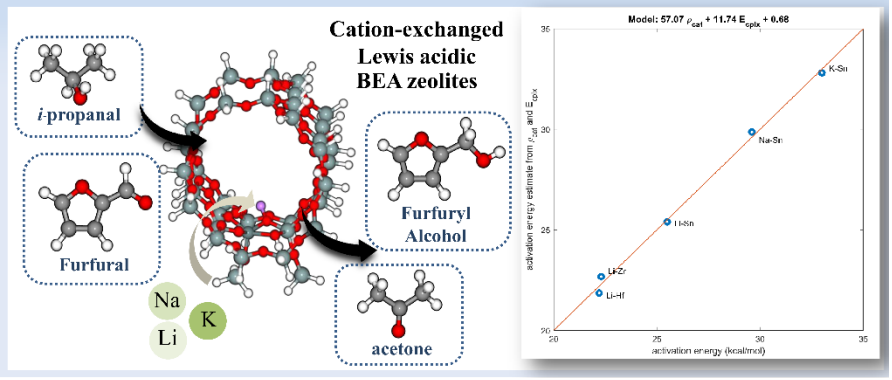

Figure 1. The optimized geometry of i-carrageenan on graphitic nitrogen-doped graphene.

Keywords: Furfural, Furfuryl Alcohol, *i*-propanol, Hydrogenation, Zeolites,.

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Theoretical investigation on gas sensing properties of a MnN4 moiety embedded graphene (MnN4-graphene)

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ABSTRACT

Gas sensors play a significant role in environmental monitoring, industrial safety and medical diagnosis. It is thus important to develop gas sensor that is able to detect a target gas molecule selectively and sensitively. In this work, we employed the PBE density functional with the projector augmented-wave (PAW) method to investigate the adsorption behaviour of environmental gas molecules including CO, CO_2, NO, NO_2, N_2O, SO_2, NH_3, H_2S, CH_4, O_2, H_2 and N_2 on a MnN4 moiety embedded graphene (MnN4-graphene) and their effects on electronic and magnetic properties of the MnN4-graphene. The calculations show that MnN4-graphene chemically adsorbed with CO, NO and NO_2 gases but weakly interact with the other gases. The strong interactions between the adsorbed molecules and the MnN4-graphene induce significant change in electronic and magnetic properties of MnN4-graphene. The magnetic moment of MnN4-graphene is dramatically altered by NO and CO adsorption and it is moderately changed by NO_2 adsorption. Based on selectivity to particular gas and distinct change in magnetic property, MnN4-graphene is a promising magnetic gas sensor for detection of NO and CO toxic gases. In addition, this work is demonstrating the influence of gas adsorption on magnetic property of heteroatom-doped graphene which would be beneficial for further development of graphene-based magnetic materials for gas sensing applications.

Keywords: Graphene-based gas sensors, gas adsorption and DFT.

Design a Better Metalloporphyrin Semiconductor: A Theoretical Studies on the Effect of Substituents and Central Ions

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ABSTRACT

We have studied the effects on central metal and substituent group on the complex compounds metalloporphyrin as a semiconductor material. Cd^{2+}, Hg^{2+}, and Pt^{2+} were chosen as the central metal to see the effect of the elements on the nature of the group and the same period and reviewed the effect of substituent groups pull and push the electrons to the electronic properties of complex metalloporphyrin. The DFT/B3LYP/LANL2DZ and TD-DFT calculation were used to generate the optimized structure of, electronic and photophysical properties. The parameter is an Eg complex compound, DOS, and electronic absorption spectra. The calculations showed electron donating complexes tend to be better as a semiconductor because it lowers Eg complex compounds metalloporphyrin, NH2 group gave the smallest Eg compared to other groups.

Substituent Group	Cd			Hg			Pt		
	HOMO	LUMO	Eg	HOMO	LUMO	Eg	HOMO	LUMO	Eg
H	-5.37	-2.51	2.86	-5.34	-2.49	2.85	-5.65	-2.47	3.18
F	-5.79	-3.16	2.63	-5.76	-3.14	2.62	-6.01	-3.09	3.01
I	-5.69	-3.14	2.55	-5.67	-3.14	2.53	-5.93	-3.03	2.9
NO_2	-7.02	-4.18	2.84	-7.13	-4.53	2.6	-4.58	-1.62	2.96
NH_2	-3.47	-1.67	1.8	-3.46	-1.67	1.79	-3.76	-1.65	2.11
CH_3	-4.9	-2.33	2.57	-4.87	-2.32	2.55	-5.16	-2.23	2.93

Table 1. Orbital energy level and band gaps of the complex in eV.

Keywords: Energy band gap, Metalloporphyrin, DFT

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3D-QSAR and molecular docking of xanthone derivatives as HIV-1 reverse transcriptase inhibitors

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ABSTRACT

Structure quantitative structure–activity relationship (QSAR) studies were performed on the human immunodeficiency virus type-1 reverse transcriptase (HIV-1 RT) with 17 xanthone derivatives using comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) implemented in the SYBYL-x2.0. The best CoMFA and CoMSIA the models have only low to moderate predictive power since this method cannot explain interactions in xanthone derivatives. Therefore, the molecular interaction of the best studied active xanthone (γ-mangostin) at the non-nucleoside binding site of the HIV-1 RT wild type structure (3v81.pdb) was investigated by means of molecular docking, using AutoDock Vina. Molecular docking provides the highest binding affinity as -8.9 kcal/mol displaying hydrophobic interactions between γ-mangostin and TYR181, TYR188 and TRP 229. Accordingly, the QSAR and molecular docking results can be combined to gain insight into the structural requirements of HIV-1 RT inhibitors in a class of xanthone derivatives and provide a gainful guideline to design and predict novel and highly potent compounds for HIV-1 RT inhibitions.

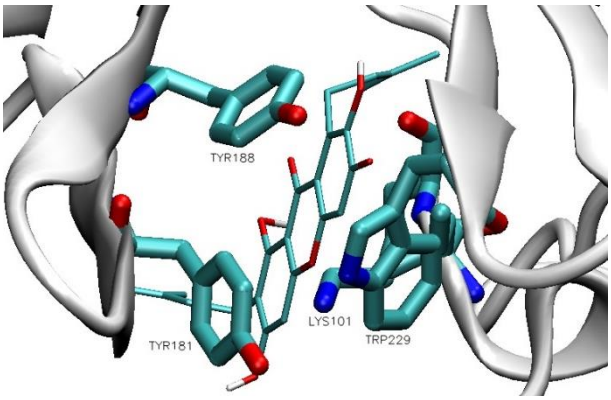

Table 1. γ-mangostin and the active residues at the non-nucleoside binding site of 3v81.pdb.

Keywords: QSAR, molecular docking, xanthone, HIV-1 RT.

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Series of D-π-A-π-A system based on isoindigo dyes for DSSC: Combined Experimental and DFT-TDDFT Computational Study

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The designs of metal-free dyes based on isoindigo have been investigated with density functional theory (DFT) and time-dependent DFT (TDDFT) calculations to improve efficiency of dye sensitized solar cells. The results indicated that **TIDP** exhibits a slow charge recombination and good intramolecular charge transfer mechanism from donor to acceptor. Moreover, the effect of dihedral angle of dye absorbed on TiO_2 indicate a smaller dihedral angle of **TIDP** leading to increase injection of electron and increased amount of dye adsorbed on TiO_2. These results suggested that the substitution of π-linker of **TIDP** can improve the abilities of electron injection as well as photoelectric properties of dye-sensitized solar cells.

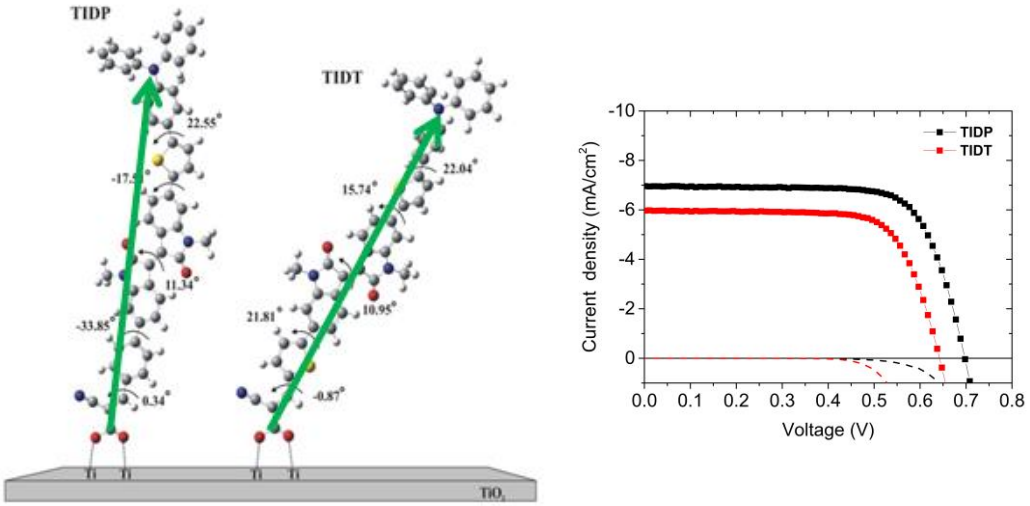

Table 1. Molecules of **TIDP** and **TIDT** with the electronic properties

Keywords: Isoindigo, Dye sensitized solar cells, D- π-A-π-A, DFT

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The Spatial Resolution in Fluorescent-Particle Tracking Affected by Motion Blur

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ABSTRACT

The spatial resolution of the tracking of mobilizing particles was studied by using simulated fluorescence images related to the movement of particles and the camera framerate. The image consists of multiple fluorescence spots related to the position of particle at different time, which was calculated using the random-walk simulations. The displacement of particle per frame that is higher than detector pixel size creates the distortion of fluorescence spot. The localization uncertainty rapidly increases when the averaged particle displacement per frame is higher than the deviation of typical fluorescence spot. The results could be used as the guidelines of an experimental setup, that is, by adjusting a camera framerate for tracking a mobilizing particle with optimal root-mean-squared displacement per frame, the motion blur effect can be suppressed, therefore, the spatial resolution could be improved.

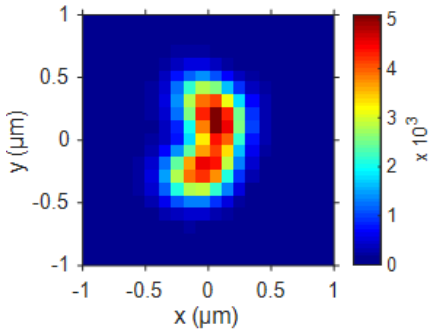

Figure 1. Fluorescence image generated by fluorescence spots corresponding to the simulated particle trajectories.

Keywords: Spatial resolution, motion blur, particle tracking, fluorescence imaging, random-walk simulation, Brownian diffusion

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Dimer Interactions of Hv1 Proton Channel in Resting State by Molecular Dynamics Simulations

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ABSTRACT

The voltage-gated proton-selective channel (Hv1) is made of four transmembrane segments (S1-S4) and cytoplasmic C-terminal helix. The S1-S4 helices assemble to form a voltage-sensing domain (VSD) and a proton permeation pathway. Although Hv1 has been found to be a dimer in biological membranes, the isolated Hv1 can be functional independence. Crystal structures of Hv1 channels in the resting state have revealed that the S4 helix and C terminal domain (CTD) in the two monomers are in closed contact across the dimer interface. Interactions between these regions play important role for the stability of the dimer and channel activity, but are not fully understood. Here, all-atom molecular dynamics (MD) simulations of Hv1 channel in the resting state in a phospholipid bilayer have been performed to explore structure, dynamics and detailed intersubunit interactions of Hv1. The results show that the flexibility between the two VSDs is different. The major contact between the two monomer are located at the C-terminal domain.

Keywords: Hv1, molecular dynamics simulation (MD).

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Adsorption of hydrogen sulfide over metal exchanged zeolite clusters: A density functional theory study

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ABSTRACT

In the past century, hydrogen sulfide (H_2S) is one of the most common compounds, which can be produce in many industrial processes such as coal gasification, residual oil gasification, and fuel cell applications. The air contamination of H_2S caused the acid rain, which directly influences the living of human, animal and plant, while the contamination of H_2S in the fuel causes the corrosion of the engine and their accessories resulting in high maintenance cost. Therefore, the removal of H_2S from fuel is necessary in order to prevent air pollution or to obtain the clean fuel. Desulfurization is one of the most important hydrotreating processes in Coal Conversion that use for removal of sulfur compound from the Coal-derived gases. In this research, the H_2S adsorption on additional framework with cations of metals (Cu and Ag) in zeolite cluster was investigated. In this work, the density functional theory (DFT) were performed by B3LYP functional combined with LanL2DZ and 6-31G (d, p) basis set using Gaussian 09 program. The result showed that hydrogen sulfide adsorption on the metal-zeolite clusters, the adsorption energies were in the range of -0.41 to -0.95 eV. The adsorption data in this study will be substantially beneficial for the improvement of desulfurization reaction mechanism.

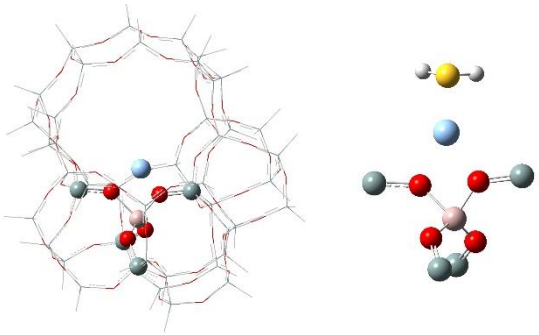

Figure 1. Optimized geometry of adsorbed H_2S on zeolite cluster

Keywords: desulfurization, Density Functional Theory (DFT).

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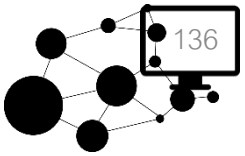
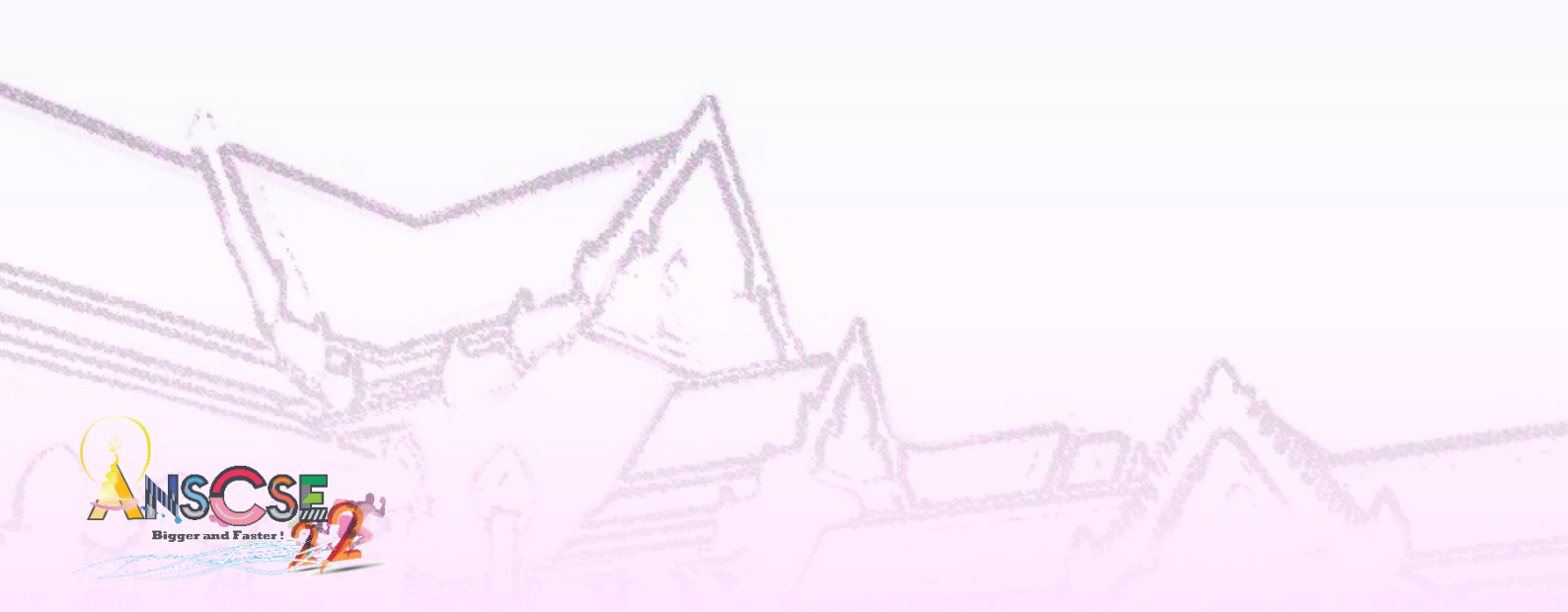


III) Computational Physics, Computational Fluid Dynamics and Solid Mechanics



Self-trapped hole in $BaTiO_3$

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ABSTRACT

Barium titanate ($BaTiO_3$) is a promising material for many technological applications, including multilayer ceramic capacitors, gate dielectrics, photocatalyst, and holographic storage.[1-3] Charge localization, in the form of small polaron is expected to crucially affect its electronic and optical properties. In this talk, we present our calculated results for the behavior of hole in the valence band of $BaTiO_3$ using density-functional calculations based on the screened hybrid-functional proposed by Heyd, Scuseria, and Ernzerhof (HSE06).[4] We find that holes tend to self-trap, localizing on individual O atoms and causing local lattice distortions, forming small hole-polarons. This takes place even in the absence of intrinsic defects or impurities. The self-trapped hole (STH) is more energetically favorable than the delocalized hole in the valence band. The calculated emission peak energy corresponding to the recombination of a conduction band electron with a STH can explain the observed photoluminescence at low temperatures.[5] The stability of the STH, its migration barrier, and related emission peak is then compared to that in $SrTiO_3$.

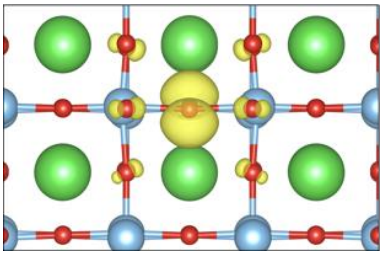

Figure Hole localization on an O atom in $BaTiO_3$.

Keywords: Small polaron, Barium titanate, Density-functional calculations

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After finishing his Ph.D. in Physics in 2009, Assist. Prof. Pakpoom Reunchan has done his postdoctoral research at APCTP in Korea and NIMS in Japan during 2009-2012. He has joined Department of Physics, Faculty of Science, Kasetsart University since 2012. His current research focuses on defect and doping physics and chemistry in complex oxides. His current H-index is 12 with over 1000 citations.

First-Principles Study of Two-Dimensional Materials for Nanoelectronics

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ABSTRACT

Nowadays, the accelerating pace in the race for envisioning new technological applications in many fields affecting human life has brought an increasing need for new a more reliable multi-functional nano-materials. Among all nanostructured materials, two-dimensional (2D) materials have been anticipated as one of the most promising alternatives to replace silicon in the electronic industry. The separation of a single graphene sheet has been performed by the group of Andre Geim and Konstantin Novoselov in 2004. Since then there has been tremendous interest in new 2D structures with diverse chemical compositions. As the building blocks for the design of electronic components, these new kinds of materials are expected to change radically the way every person in our society.

As important as these materials are for the new technological revolution, it is important to understand their structure, physical and chemical properties down to the most fundamental level, unveiling the transport mechanisms at an atomistic level. I will discuss the state of art methods using a combination of the density functional theory (DFT) and non-equilibrium Green's functions (NEGF) now available for performing quantum electronic transport simulations. We can simulate prototypical 2D nanostructure devices (graphene, silicene and phosphorene) for various applications; for example, gas sensors[1], DNA sequencing[2,3] and spintronics devices[4].

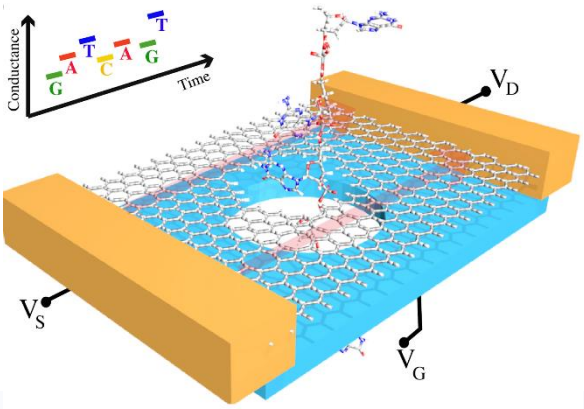

Figure Schematic setup for a DNA sequencing device constructed by embedding line defects around a nanopore in graphene connected to a source and drain (in yellow color), with an additional gate electrode (in blue color) below[3].

Keywords: Nanoelectronics; Two-dimensional materials; Density Functional Theory

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4. W. Rotjanapittayakul *et al*. *Sci. Rep*., 2018, **8**(1), 4779.

Jariyanee studied Physics (B.S) at Chiang Mai University and at Mahidol University in Thailand where she earned a Master's Degree on "Exchange interactions in the metallic compounds GdCo4-xNixAl" with Prof. I-Ming Tang. She started her Ph.D. at Uppsala University with Prof. Rajeev Ahuja. Her thesis work focused on the electrical conduction properties in nanoscale systems. After defending her PhD thesis, she has worked at Nakhon Phanom University since January 2012.

2D van der Waals Heterostructures for Nanoelectronics

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ABSTRACT

Van der Waals heterostructures (vdWHs), a new class of 2D layered materials made of a vertically controllable assembly of various 2D monolayers held together by van der Waals forces, have attracted a great deal of attention due to their promise to offer novel physics and versatility that are not achievable in individual 2D crystals. This talk presents recent advances on vdWHs and their potential applications in nanoelectronics. First, fabrication approaches, i. e., mechanical transfer and chemical vapor deposition growth are briefly discussed. Afterwards, the intrinsic band alignments originated from combining different 2D materials are introduced. In addition, devices applications such as light-emitting diodes (LEDs) and photodetectors are exemplified. The final part of the talk is devoted to the theoretical study of the fundamental aspects of hexagonal boron nitride (*h*-BN) and the recent allotrope of phosphorus (blue phosphorene, BlueP) vdWH. It is revealed that this hybrid material forms a straddling type I band offset where the band edges exclusively belong to BlueP. This feature enables *h*-BN to act as a protective coating material to resolve the air instability of BlueP. Furthermore, substitutional doping of C into *h*-BN (*h*-BCN) at a suitable concentration induces *h*-BCN–BlueP into a staggered type II band offset. The type II alignment triggered by the intensified built-in electric field across the sheets implies the accelerated carrier mobility and the suppressed recombination of photo-generated electron-hole pairs. These major benefits can pave the way for the potential functionality of h-BCN–BlueP for efficient photovoltaic devices.

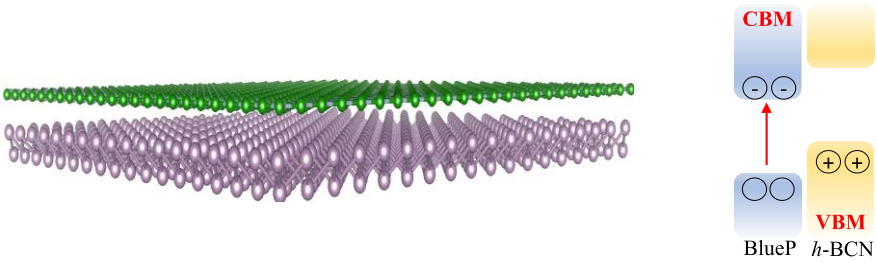

Figure 1. Atomic structure of h-BN/BlueP vdWH and its band offset diagram [3].

Keywords: van der Waals heterostructures (vdWHs), blue phosphorene, hexagonal BN.

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Essence of Correlation Energy

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ABSTRACT

The correlation energy comes from the many-particle interaction among electrons in the system. Its effect is very important in the fields of condensed matter physics, physical chemistry and computational chemistry. I will discuss the essence of the correlation energy; how it can be measured from the experiment, how it can be computed and modelled theoretically. Recently, there exists the celebrated Chachiyo formula [1] for the uniform electron gas. I will try to relate this beautiful formula to the results from quantum field theory and extract its parameters from the first principle. At the end of my talk, I will show some exciting results on the new physics of materials under high pressure in which the correlation energy is a bit more complicated than that in the uniform electron gas. The examples include the structural phase transition in strontium [2], the superhard behaviour in carbon nitride methanediide [3], and recent findings in calcium, as seen in Figure 1.

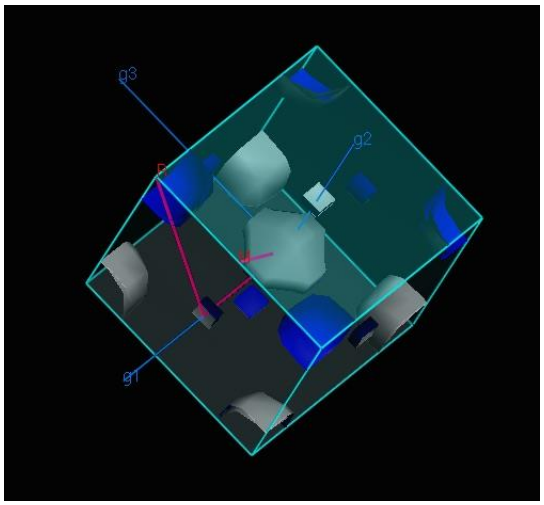

Figure 1. Fermi Surface of Calcium

Keywords: Correlation Energy, Chachiyo Formula, Materials under High Pressure

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Dr.Udomsilp Pinsook received his Ph.D. from the University of Edinburgh, UK in 1999. He is now working as a lecturer in the department of Physics, Faculty of Science, Chulalongkorn University, Thailand. His recent research works are concentrated on the new physics of materials under high pressure using the density functional theory, quantum many-particle physics and path integral method.

Inflation from Supersymmetry Breaking

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ABSTRACT

We explore the possibility that inflation is driven by supersymmetry breaking with the superpartner of the goldstino playing the role of the inflaton. These models are characterized by an inflationary plateau around the maximum of the scalar potential, with the inflaton rolling down to a minimum describing the present phase of our Universe. The proposed models agree with cosmological observations.

Keywords: Cosmology, Inflation, Supersymmetry

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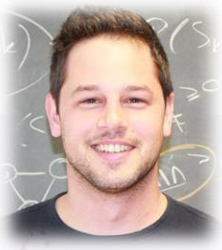

Rob Knoops is a researcher at the “CUniverse” project at Chulalongkorn University. His research focuses on phenomenological aspects of supergravity and cosmology. He obtained his PhD at the Catholic University of Leuven, and has worked at CERN and Geneva University.

The response of electronic properties of monolayer to elastic strain and the stacking stability of bilayer C_2N

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ABSTRACT

Two-dimensional (2D) monolayer honeycomb structures offer remarkable properties and are promising materials for future applications. Recently, a new 2D graphene-like sheet: C_2N, was synthesized via a simple wet-logical reaction.[1] In this work, we will reveal the electronic and mechanical properties of recently synthesized monolayer C_2N based on first-principles calculations. In 2D materials, the mechanical strength is represented in term of in-plane stiffness and Poisson's ratio in harmonic region. The limit of structural deformation under applied strain can be evaluated by using the electron localization function (ELF). Afterward, the electronic properties under both uniaxial and uniform strain in the elastic range will be study. In the preliminary research stage, we found that the band gap decreases when the strain is applied along zigzag or/and armchair direction.

Then, we study the stability and electronic properties of bilayer C_2N. According to previous study,[2] in order to stack monolayer into bilayer, there are three high symmetric stacking configurations namely as AA-, AB- and AB'-stacking. For the AA-stacking, the top layer is directly stacked on the bottom layer. Furthermore, AB- and AB'-stacking can be obtained by shifting the top layer by a half of the unitcell from AA-stacking along zigzag direction and by one third of the unitcell along armchair direction respectively. By using first-principles calculations, we calculated the stability of AA-, AB- and AB'-stacking bilayer and their electronic band structure. We found that AB-stacking is the most stable and has the highest band gap among AA- and AB'-stacking, which appeared to agree with previous study. Nevertheless, we furthermore examine the sliding barriers and energy profiles between bilayer stacking order when we applied uniform strain. From energy profiles, we interestingly found that the most stable positions are shifted from the high symmetry AB-stacking. In band structure calculation details, the electronic band structure of bilayer C_2N can be modified according to the ways of shifting.

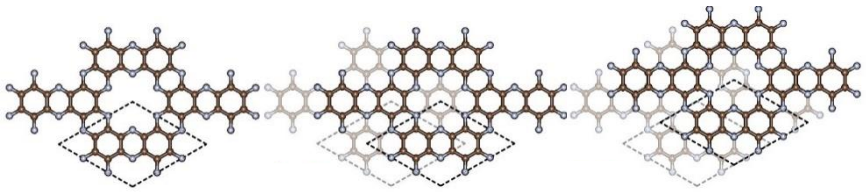

Figure (a, b, c) AA-, AB-, and AB'-stacking structures of 2x2 supercell bilayer C_2N, respectively. The C atoms are represented by brown balls and the N atoms are represented by grey balls.

Keywords: C_2N, First-principles calculation, strain, bilayer stacking

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Atomistic tight-binding theory in alloy semiconductor nanostructures

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ABSTRACT

In the combination with atomistic tight-binding theory (TB), an empirical bowing parameter and the widely used virtual crystal approximation (VCA), the theoretical investigations of alloy nanocrystals with the experimentally synthesized sizes and compositions (x) are reported. [1, 2] A good agreement is achieved between the tight-binding values and the experimental data. In term of the potential application, the polarized entangled photon pair produced by the biexciton (XX) - exciton (X) - ground state (0) cascade procedure [3] is studied. However, the entanglement of the photon pair is devastated by the fine structure splitting (FSS) introduced from the electron-hole exchange interaction. Using the configuration interaction description (CI), I demonstrate the control of the excitonic fine structure splitting by engineering the alloy elements and sizes. Finally, the present systematic study from this atomistic model is one of the most important milestones on the road to provide the understanding of the structural and optical properties and a complete tactic to design the nanodevices based on the alloy semiconductor nanostructures.

Keywords: Tight-binding theory, Alloy, Nanocrystal.

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First-Principle Study of Strain-Induced Band Gap Tunability of Two-Dimensional Transition Metal Dichalcogenides MX_2 (M = Mo, W; X = O, S, Se, Te)

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ABSTRACT

Recently, two-dimensional transition metal dichalcogenides (2D-TMDs) have attracted much research interest and been realized as a new class of 2D materials with excellent properties. The 2D-TMDs can be fabricated by exfoliation for high quantity [1] and chemical vapor deposition (CVD) for large scale [2]. When bulk TMDs are rescaled to a few layers, they show extraordinary electrical [3], optical [4] and mechanical [5] properties. Especially in Group-VI TMDs, most of them are direct-band-gap semiconductors with tunable band gap, making them suitable for electronic [3, 6] and optoelectronic applications [6, 7]. Another interesting property of 2D-TMDs is their flexibility as they can withstand strain up to 10% without deformation [5]. It has been experimentally confirmed by various techniques, such as substrate thermal expansion for biaxial strain [8] and substrate bending for uniaxial strain [9], that strains play important roles to control the electronic and optical properties of the 2D-TMDs. In this work, we theoretically study the strain-induced band gap tunability of Group-VI TMDs MX_2 with M = Mo, W; and X = O, S, Se, Te using density functional theory (DFT) with the consideration of biaxial and uniaxial strains into account. The results show that the band gap modulation is more sensitive to the biaxial strain. This finding is consistent with the experimental studies of MoS_2 [9, 10]. We also show that a wide range of band gap can be achieved by applying strains ranging from -10% to 10%. Consequently, our results provide guidelines for application of Group-VI TMDs by employing the strain engineering.

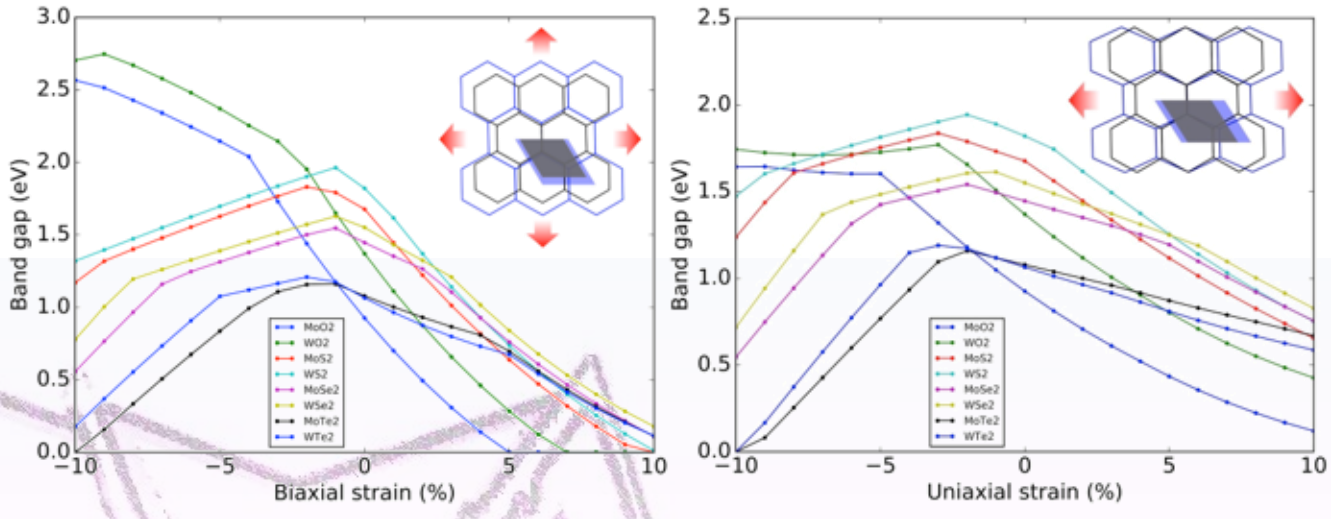

Figure Band gaps of single-layer MX_2 (M = Mo, W; X = O, S, Se, Te) under biaxial strain (left) and uniaxial strain (right). The insets illustrate effects of the applied strains resulting in modulation of a unit cell (blue) from as compared with an unstrained one (black).

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Electronic and Optical Properties of Silver Chloride Photocatalyst by First Principles calculation

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ABSTRACT

In this work we study the electronic and optical properties of the photocatalytic materials AgCl. Based on Density Functional Theory (DFT) with Generalized Gradient Approximation (GGA), optimized lattice parameter, band gap, density of states, and dielectric functions of the bulk AgCl are calculated. To accurately determine the AgCl band gap, its band energies are corrected by using the GW and QPscGW method. Further to the DFT-GGA and GW electronic band structure calculations of the bulk AgCl, the dielectric functions, which manifest the optical properties, are calculated by random phase approximation (RPA) and Bethe-Salpeter equation (BSE), that includes the electron-hole correlation effect and show strong excitonic peaks. Then, we compare our theoretical results with the available different methods and finally discuss the key issues that influence the photocatalytic properties.

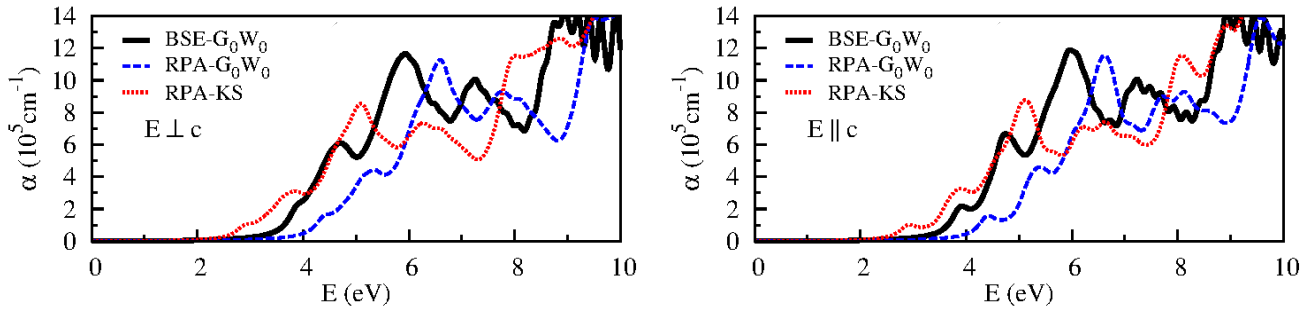

Figure Absorption coefficient of the AgCl

Keywords: Density Functional Theory, Electronic Structure, Bethe-Salpeter equation, photocatalytic

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Predicting Coefficient of Linear Thermal Expansion of Carbon Fiber/Graphene Nanoplatelet/EPON862 Hybrid Composites: Multiscale Modeling

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ABSTRACT

Carbon Fiber/Epoxy composites are already used for lightweight components in aerospace applications due to its relatively high specific strength and high specific stiffness. By replacing the heavier materials like metals, the lighter vehicles consume less fuel. Even the composites have many advantages, improvement of this materials is still needed, especially, the matrix or the binder. Recently, graphene nanoplatelet (GNP) [1] was introduced into the epoxy region to increase the effective elastic properties of GNP/Epoxy composites by using multiscale modeling including molecular dynamics (MD) and micromechanics. For GNP/Carbon Fiber/Epoxy hybrid composites, the effective elastic modulus increased in transverse direction (radial direction) with increase amount of GNP and with the better GNP dispersion.

Coefficient of Linear Thermal Expansion (CLTE) is an important thermomechanical property. The CLTE indicates how the size of materials changes in each direction when the materials are exposed to different temperatures. For Carbon Fiber/Epoxy composites, their axial CLTE is very small or close to zero. With the reduction of axial CLTE, the Carbon Fiber composites can decrease the thermal sag of high voltage cable [2]. On the other hand, the transverse CLTE is still large meaning that the materials could normally expand in transverse direction. In case of GNP inclusion, the CLTEs of composites have not been investigated, yet.

In this research [3], the MD models of GNP/Epoxy systems were obtained from Cameron Hadden [1] including 1, 2, 3, and 4-layer(s) of GNP/Epoxy models. The CLTEs of these models were determined by using heating up and cooling down method in MD simulation with the Large-scale Atomic/Molecular Massively Parallel Simulators (LAMMPS) [4]. The resulting CLTEs were randomized by using Craft and Christensen equation. The effective CLTEs of GNP/Epoxy composites and GNP/Carbon Fiber/Epoxy hybrid composites were calculated in Micromechanics Analysis Code based on the Generalized Method of Cells (MAC/GMC) [5] by varying the volume fraction of GNP. The MAC/GMC software uses repeating unit cell (RUC) shown as Figure to represent the model of GNP/Epoxy composites.

The normalized CLTEs of GNP/Epoxy composites are shown in Figure. The normalized CLTE is ratio between CLTE of GNP/Epoxy and the CLTE of neat epoxy. The normalized CLTEs decrease with increased the volume fraction of GNP. The perfect GNP dispersion (1-layer GNP) model has the lowest normalized CLTE. The similar trend happens to the transverse CLTE of GNP/Carbon Fiber/Epoxy hybrid composites. However, the axial CLTE of the hybrid composites increases with increased GNP volume fraction. For GNP volume fraction less 10%, the perfect GNP dispersion provides the highest axial CLTE of the hybrid composites.

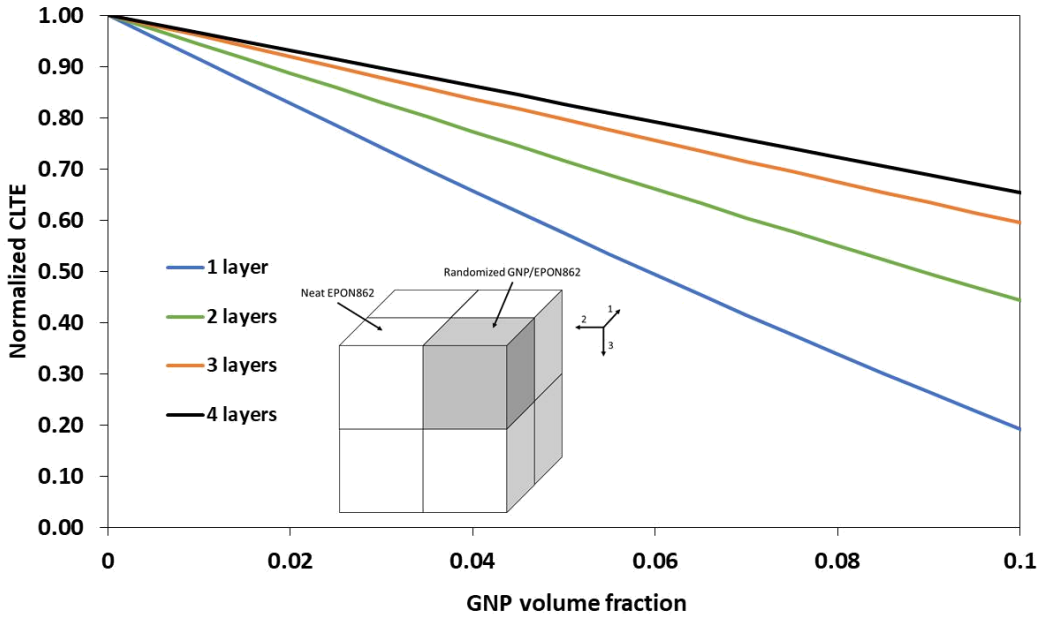

Figure Representative RUC in MAC/GMC and the plot of normalized CLTEs of GNP/Carbon Fiber/Epoxy hybrid composites as the function of GNP volume fraction.

The normalized CLTEs of GNP/Epoxy composites are shown in Figure. The normalized CLTE is ratio between CLTE of GNP/Epoxy and the CLTE of neat epoxy. The normalized CLTEs decrease with increased the volume fraction of GNP. The perfect GNP dispersion (1-layer GNP) model has the lowest normalized CLTE. The similar trend happens to the transverse CLTE of GNP/Carbon Fiber/Epoxy hybrid composites. However, the axial CLTE of the hybrid composites increases with increased GNP volume fraction. For GNP volume fraction less 10%, the perfect GNP dispersion provides the highest axial CLTE of the hybrid composites.

Keywords: Molecular Dynamics, Graphene, Composite, Epoxy, Carbon Fiber, Thermal Expansion, Micromechanics

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Matrix Tridiagonalization Methods for 3D Finite Element Analysis of Free Vibration

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ABSTRACT

Mechanical resonance is the phenomenon that a mechanical system vibrates at larger amplitude when the oscillation frequency corresponds to one of the system's natural frequencies. This leads to violent motion and potentially catastrophic failure of structures such as bridges, buildings and machines. To avoid mechanical resonance, a vibrating system needs to be designed such that its working frequency interval is sufficiently far from its natural frequencies.

Natural frequencies of a mechanical system are normally determined from free vibration analysis [1]. For a real engineering system, it typically consists of 3D complex geometries and therefore the free vibration analysis is commonly performed by the finite element method. Regarding the finite element derivation of 3D free vibration problems, the mass and stiffness matrices are conventionally transformed into a single standard-form matrix. The standard-form matrix is subsequently solved for eigenvalues and eigenvectors which are natural frequencies and corresponding mode shapes, respectively. The matrix of a 3D free vibration problem usually has a relatively large size. Therefore, it requires large computer memory and long time to solve this matrix. To reduce computational resources used, the matrix is transformed into the tridiagonalized form (containing non-zero elements only on the main diagonal, and the first diagonal below and above the main diagonal) by a tridiagonalization algorithm.

The most common tridiagonalization method for relatively large matrices is the block Lanczos method [2]. Nevertheless, the matrix could lose its orthogonality during the block Lanczos operation resulting in spurious solutions [3]. To stabilize the block Lanczos algorithm, a componentwise technique for detecting and fixing the orthogonality loss has been proposed and demonstrated on general eigenvalue problems [3]. The present study investigates the effectiveness of this orthogonality fixing scheme for 3D free vibration problems. In this work, we developed three computer programs for 3D finite element analysis of free vibration by using three matrix tridiagonalization methods: (1) the conventional block Lanczos method (BL), (2) the block Lanczos method with the orthogonality fixing scheme (BLO) and (3) the Householder method [4]. The three methods are compared in terms of solution accuracy and computational time.

The results in this work show that the BL method suffers two problems which are repeated natural frequency values and "pseudo modes". These problems are caused by the loss of matrix orthogonality during tridiagonalization causing rounding errors in subsequent steps of computation. This study also reveals that the BLO method gives accurate solutions for 3D free vibration analysis. As for the Householder method, it does not experience the loss of matrix orthogonality and its accuracy is similar to that of the BLO method. In terms of computational time used, the BLO method uses significantly more time than the BL method does because some part of computer resources was used for the orthogonality fixing operation. Compared to the Householder method, the BLO method uses significantly less computational time for relatively-large matrices (Fig. 1). Therefore, the BLO method is a suitable choice for the matrix tridiagonalization operation in 3D free vibration analysis.

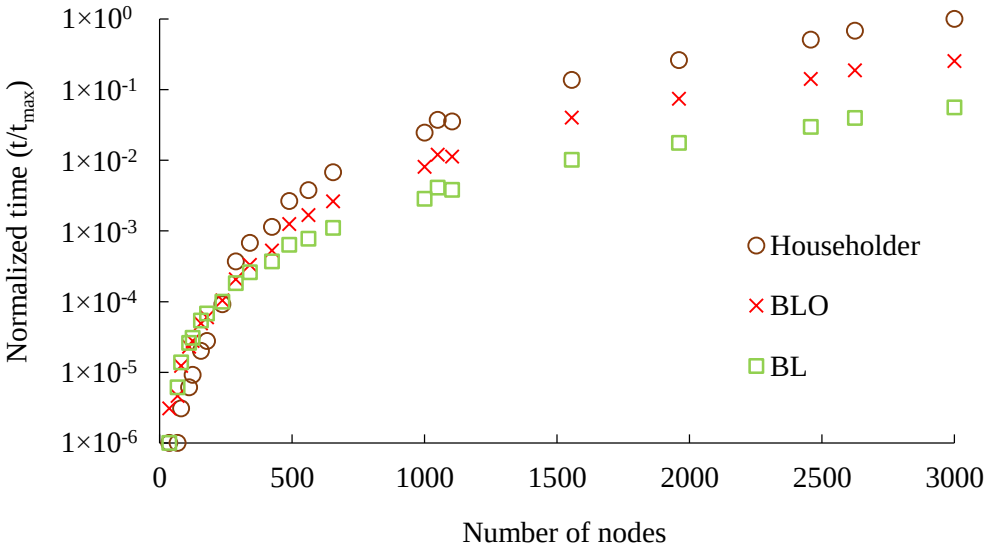

Figure Computation time used by different tridiagonalization methods.

Keywords: Matrix Tridiagonalization, Eigenvalue Problem, Free Vibration, Block Lanczos, Orthogonality.

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Identify Transient Sources from GOTO Sky Survey Data with Clustering Method

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ABSTRACT

The Gravitational-wave Optical Transient Observer (GOTO) Sky Surveys project has an objective to identify optical counterparts to gravitational wave detection by detecting all transient sources in the sky. The large amounts of images data from the sky every night will be processed and analysed in order to classify 40-million observed source samples. It is impossible to identify and classify new bright sources from such a big number of samples by human only. Therefore, machine learning is the important part for this project. Classification was the first technique that was implemented to solve this problem. However, there are several shortcomings in the solution from the classification due to the extremely imbalance of the data, where the number of identified sources is very big compared with the transient one. In order to solve the shortcomings, some clustering methods such as K-Means, Agglomerative and DBSCAN were introduced and their results were evaluated with several clustering indices. We will discuss the results and their applications in GOTO project in the meeting.

Keywords

Gravitational-wave detectors, Transient source detection, Data clustering, Imbalance data

Machine Learning system mimicking student's choice in Particle Data Analysis laboratory activity

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ABSTRACT

A machine learning system is designed to supplement a Physics laboratory activity for undergraduate and high school students in which a student classifies collision events which contain two muons decaying from J/psi meson within CMS detector. The system is designed in such a way that it can mimic the student's classification, and after its training is complete, the system can help the student classify a subset of collision events which the student did not classify. This system can allow the student to spend less time by classifying a smaller subset of events from the entire collection. In this project, a cut-based classifier is also developed to illustrate the "perfect classification" to the student, and the student is able to compare his/her classification results with. The results from the machine learning classifier is not expected to be identical to cut-based classifier, since the classifier's aim is to mimic the student and not following the perfect classification rule.

Keywords: CMS Outreach, Machine Learning

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First-principles study of defects in Bi and Al doped orthorhombic $PbZrO_3$

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ABSTRACT

One of the most important ceramic materials for many technological applications is lead zirconate (PZO) due to its antiferroelectric property. Lead-free ferroelectric materials are widely carried out by reason of the toxicity of Pb. The incorporation of bismuth aluminate (BAO) into PZO has been reported that it could stabilize the antiferroelectric property in a wide temperature range and reduce the Pb content. In this work, defects in Bi and Al doped orthorhombic-PZO have been investigated the structural and electronic properties, and formation energies using first-principles calculations based on Density Functional Theory (DFT). Our calculated results of defect formation energies showed that Bi atom can substitute not only on the Pb site (A-site), but also on the Zr site (B-site) depending on the Fermi level and the crystal growth condition. Whereas Al atom prefers to substitute only on the Zr site. In addition, we found that the binding energies of Bi_{Pb}-Al_{Zr} and Bi_{Pb}-Bi_{Zr} complex defects are very small (~0.1 to 0.2 eV). This indicates that the majority of Bi and Al atoms in orthorhombic-PZO should exist in the form of isolated substitutional defects.

Keywords: First-principles calculations, DFT, Orthorhombic $PbZr_3$, PZO..

Surface Structure Determination of TiO_2(110)(1x2) Dynamic Scattering of Electrons in LEED-IV

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ABSTRACT

Annealing of a TiO2(110) sample in UHV leads to bulk reduction. In addition to bulk modification, the surface also changes in response to this thermal treatment. Initially, it exhibits a (1x1) termination, but undergoes reconstruction to a (1x2) added row phase as the degree of bulk nonstoichiometry increases. Notably, there are two types of (1x2) reconstruction, a simple (1x2), and an x-linked (1x2), with the latter forming at higher degrees of bulk reduction. More precisely, the x-linked (1x2) surface should be described as a (nx2) reconstruction, as it consists of (1x2) added rows with a somewhat irregular array of superposed x-linked rows. The goal of this work is to develop dynamic scattering of electrons code named SATLEED to determine the structure of the x-linked (1x2) reconstruction, using LEED-IV measurements. The analysis indicates that the x-linked TiO_2 (110)(1x2) reconstruction consists of Ti_2O_3 added rows. Consistent with SXRD, two coexisting differently relaxed Ti_2O_3 added rows have been found. Slight differences between the surface coordinates deduced from LEED-IV and SXRD analysis may be due to different levels of bulk reduction when the samples are prepared. Further calculations show possibilities of mixing states of these reduction or even asymmetric model of this surface.

Keywords: LEED-IV, SATLEED, dynamic scattering, electron diffraction**,** TiO_2

Meshless local Petrov-Galerkin (MLPG) method for HIV model

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ABSTRACT

In this paper, we present the numerical approximation of the HIV model by Meshless local Petrov-galerkin (MLPG) method and finite difference technique. The approximation solutions of the HIV model for the spatial discretization used by the MLPG method. In the MLPG method, the moving Kriging interpolation is employed to construct a shape function which has the Kronnecker delta property. And Dirac delta function is applied in local weak form as test functions. For the temporal discretization used finite difference technique. Numerical results were compared with the approximation solution of the HIV model using the implicit finite difference method to confirm the accuracy of the proposed method. In conclusion, the results of a numerical experiment are agreed too.

Keywords: HIV model. MLPG method, Local weak formulation, implicit finite difference method.

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The Numerical Solution of Fractional Black-Scholes-Schrodinger Equation Using the MLPG Method

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ABSTRACT

This paper mainly focuses on the fractional Black-Scholes-Schrodinger equation is solved by using a numerical techniques for the option price in financial problems. The meshless local Petrov-Galerkin (MLPG) method is applied for spatial discretization. The approximation of time fractional derivative is interpreted in the Caputo's sense by a simple quadrature formula. In MLPG method, the moving kriging interpolation is applied to constructing shape function. The Kronecker delta function is chosen to be the test function for simplifying the equation. Numerical solution is compared with the semi-classical solution to verify the results. The results can be concluded that the option price from MLPG method are agreed to the semi-classical solution.

Keywords: Black-Scholes-Schrodinger Equation, Fractional Model, Meshless local Petrov-Galerkin Method, Option Pricing, Quadrature formula.

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IV) High Performance Computing, Computer Science, Mathematics and Engineering

High Performance Computing, Computer Science, Mathematics and Engineering
HPC-INV-01

Mathematics Computing in Environmental Quality for Power Plant

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ABSTRACT

Electricity Generating Authority of Thailand (EGAT) initiates to proactively surveillance environmental quality around power plants. Therefore, the stay alerted of potential environmental problems requires accurate prediction information for effective planning. The forecasting data can be obtained by using a mathematical model to simulate environmental conditions over space of surrounding area of power plant in various altitudes. As it is known that the dispersion of pollutants from sources mainly depends on velocity and direction of the wind. Thus, the mesoscale non-hydrostatics model entitled the Regional Atmospheric Modeling System (RAMS) is applied for the forecasting 168-h simulation of wind data, temperature, planetary boundary layer height (PBL) and relative humidity. In order to be computationally fast enough for the forecast period, simulations are processed with parallel computing technique on the High Performance Cluster Computer of EGAT. The simulation results were compared with observational wind speed, wind direction, and temperature from various local-based meteorological stations. The comparison shows that the modelled values are generally in good agreement with observations in both land-sea area and mountain-valley area. Nowadays, the predicted data from RAMS is using to alert the haze problem and noise nuisance over power plant area. Besides the using in environmental aspects, wind data is also used for the hourly prediction of electricity generated from wind in Lam Ta Khong area up to 7-days in advance. The all forecasting display data can be accessed from the website http://tairgle.egat.co.th.

Keywords: Mathematical Model, RAMS, Forecasting, Parallel Computing, Cluster Computer

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Dr.Rudklao Pan-Aram is a Scientist level 10 in Project Environment Division, Electricity Generating Authority of Thailand (EGAT). She graduated the doctoral degree of Energy Technology from School of Energy, Environments and Material, KMUTT. She has experiences in atmospheric and air quality model for more than 18 years.

Mathematical modeling and analysis of thermal transport for materials design

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ABSTRACT

Mathematical models can provide basic understandings and mechanistic insights to various systems. Herein, the models have been constructed to assist design a new thermoelectric material and investigate the properties, focusing on the mechanical effects to the thermal property [1, 2]. The phonon transport theory coupled with the classical mechanical theory were exploited to obtain the phonon transport in nanowires, which are under the surface stress [1] and the torsional stress [2], respectively. The lattice thermal conductivity was subsequently computed based on the tailored phonon dispersion relation. The results not only showed that the mechanical effects could engineer the phonon and the thermal conductivity, but also they guided to a new design of materials which is not limited to thermoelectric applications. In addition to the conventional approach, the new aspect of computational approach in materials design using data mining and machine learning will be also discussed.

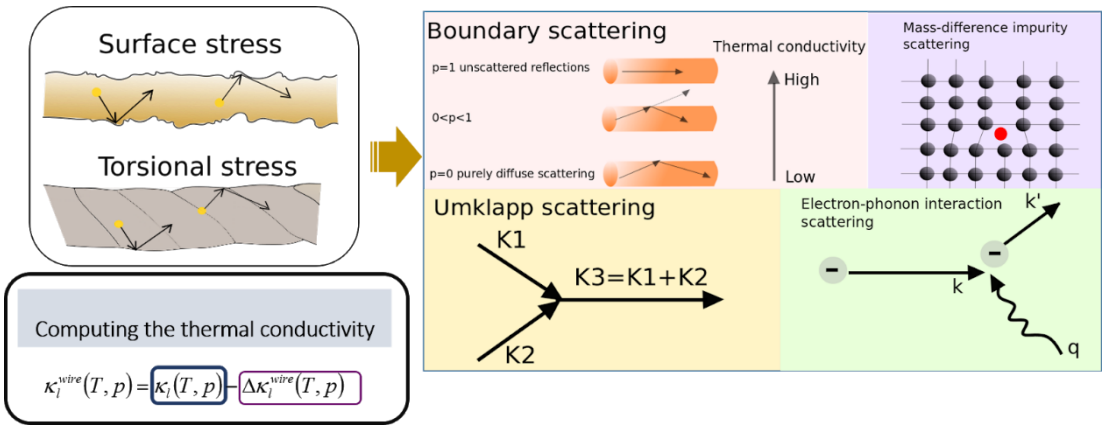

Figure Schematic diagram of computing thermal conductivity of nanowires that are subject to the surface stress and the torsional stress, and the corresponding phonon-scattering mechanisms.

Keywords: Mathematical model, Thermal conductivity, Phonon transport, Surface stress, Torsional stress

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Dr. Monrudee Liangruksa is currently a researcher at National Nanotechnology Center (NANOTEC), Thailand. She has completed her PhD in Engineering Mechanics from Department of Engineering Science and Mechanics, Virginia Tech, USA, in 2011. After completing her doctorate, she has started working at Nanoscale Simulation Laboratory, NANOTEC. Her research interests include mathematical modeling and simulation in the field of nanoscale thermal transport, nanomechanics, and applied physics with the applications in energy materials.

High Performance Computing, Computer Science, Mathematics and Engineering

HPC-INV-03

Shift/Collapse Algorithm for Fast and Scalable Many-Body n-Tuple Computation on Supercomputers

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ABSTRACT

Reactive molecular dynamics (ReMD), allowing dynamic many-body bond formation and breakage, requires significantly more computation power compared to the conventional static bond method. Recently, we developed a shift/collapse (SC) algorithm, a novel MD computation algorithm that utilizes optimal communication scheme for *n*-tuple interaction, which significantly improves computation performance of ReMD [1]. In this work, we presented two new developments of SC algorithm for broader types of ReMD. First, we used SC algorithm on neighbor list (SC-NBL), which combines advantages from reduced search space of neighbor list and optimal *n*-tuple communication scheme of SC algorithm. Implementation of SC-NBL has been verified and the simulation results have been thoroughly validated using force fields with 2- and 3-body bond-breakable interactions on SiO_2 system [2]. Second, we developed a renormalized SC algorithm (RSC) for renormalized many-body *n*-tuple computation. RSC is an essential solution to address renormalization parameters in embedded-atom method (EAM), bond-order potentials (BOPs), and conjugate gradient (CG) calculation.

Performance benchmark showed significant performance improvement of SC-NBL over the original SC algorithm with 1.33× and 3.29× speedups on small and large granularities (24 and 24,000 atoms per compute core), respectively. Large-scale benchmark indicated simulation performance of up to 267 ns/day for grain size of 24 atoms/core on 1,296 cores of Intel Xeon processors. For RSC, we observed performance improvement for polarizable charge equilibration calculation (PQEq) in reactive force-field MD (reaxFF) [3] is 5.0 times faster than the ordinary PQEq implementation. These new developments of SC highlighted an important step toward generalization of SC algorithm for general ReMD simulations.

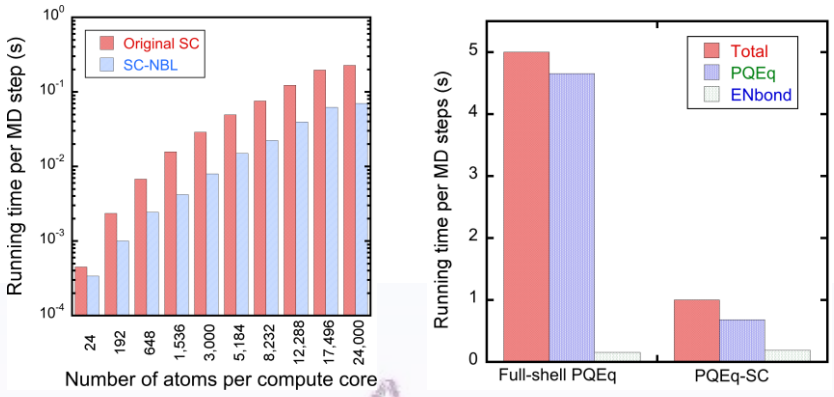

Figure 1. (Left) Running time speedup of SC-NBL over original SC algorithm (Right) Running time comparison of PQEq-SC algorithm versus the ordinary PQEq algorithm.

Keywords: Shift/collapse algorithm, Many-body potentials, Performance optimization, Molecular dynamics

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High Performance Computing, Computer Science, Mathematics and Engineering
HPC-INV-04

Computational Approaches for Pre-Clinical Study of a New Treatment Modality in Radiation Therapy

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ABSTRACT

The aim of radiation therapy is to deliver highly conformal dose to the target tumor while sparing surrounding healthy tissue from radiation damage. Proton therapy is a new treatment modality that can achieve this goal. Therefore, many radiation therapy centers worldwide, including those in Thailand, have growing interest in acquiring proton therapy systems for cancer treatment. To prepare for the shift of the treatment modality, computational approaches for planning and studying patient-specific dose distributions by proton therapy versus conventional radiation therapy using high-energy X-rays and electrons are inevitable. For such studies, treatment planning systems (TPS) and Monte Carlo simulations of radiation transport are commonly used tools in the medical physics community. Commercial TPS are usually expensive and have closed architecture that prevents users from scrutinizing or modifying physics models and algorithms behind the proton dose calculation. In contrast, most of Monte Carlo simulation codes used in radiation therapy have royalty-free licenses, but Monte Carlo simulations of radiation transport require high-performance computing resources to compromise between the accuracy and the computation time. This talk will cover (i) the recent development of the proton therapy treatment planning system PSPLAN for pre-clinical study of patient-specific proton dose distributions and (ii) the application of Monte Carlo simulations in proton therapy research.

Keywords: Radiatiton Therapy, Proton Therapy, Monte Carlo simulation, Treatment Planning System.

Dr. Thiansin Liamsuwan obtained her PhD in Medical Radiation Physics from Stockholm University, Sweden in 2012 and Diplom-Physik (integrated BSc and MSc) from University of Karlsruhe, Germany in 2008. She has solid background in development and application of Monte Carlo simulations in radiation biophysics and radiation therapy. Her current research focuses on development and application of computational approaches for accurate determination of patient-specific dose distributions received by different treatment modalities in radiation therapy

Loop prevention on Software Defined Network using Adaptive Virtual Tunnel Network

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ABSTRACT

Nowadays, cloud data center is very high complexity and requires a lot of network devices. The automate networking systems and centralize management system are needed to meet customer's expectations. Loop is a most common problem in general and enterprise network. Spanning tree protocol (STP) is a standard loop detection and recovery by drop some network links to remove loop. All network switches require pre-configuration manually. Software-Defined Networking (SDN) has solved this problem. With SDN, the control plane is removed from network device's hardware and implements it in software call SDN Controller instead. With the OpenFlow protocol [1], SDN Controller centrally control routing, network operation and each network device can be configuration centrally. OpenDaylight has feature to prevent loop called Loop remover that imitate technique from STP. Loop remover has a limitation of best path selection. In this paper, we used OpenDaylight as SDN Controller and operated features called Virtual Tenant Network (VTN) [2]. VTN provides multi-tenant virtual network on an SDN controller for single physical network resources. VTN can reduce the investment for each physical tenant network, simplifies design, implement and operate the entire complex network. Although network is designed on VTN, the data is still transferred over the physical network which can be a complicated network and cause a loop on SDN. This paper, we develop our loop prevention system based on VTN application. We provide automate loop prevention and routing management by calculate the best path by using Dijkstra's Algorithm. The packages flow generates by SDN and VTN application automatically.

Keywords: SDN, VTN, Loop, OpenDaylight.

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Resilience flow management on Software-Defined Network using Directed graph for L2 Loop prevention

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ABSTRACT

In large-scale datacentres that are dealing with thousands of computer servers, storages and network switches. The network problem happens regularly from many factors such as hardware malfunction, human errors and software errors. The network loop is a one of common problem that are occurring from human error. To prevent this problem, normal data centre run a Spanning Tree Protocol (STP) that will drop some network links to eliminate network loop with specific conditions. However, network management in large-scale datacentre very difficult and high complexity. Because of their network consist of many network switch's brand and it require a special command to management. Software-Defined Network (SDN) solve these problems by separate operation of control plane and data plane. The control plane is a part of packets flow control and policies management. The second part is data plane by performs the packet forwarding. SDN required centralize management called controller to act as software control plane. Opendaylight (ODL) is most popular SDN controller and support interfacing with GUI and REST API. ODL supported standard loop detection and prevention by using Spanning Tree Protocol (STP). STP provide mechanism to drop some network link to evade network loop. To control the network flow and forwarding direction cannot possible when using STP. In this work, we extended our program, called Spinner, to detect loop in SDN network and provide dynamic forwarding flow to every Openflow switches. The directed graph technique is used as loop detection. Spinner provide the normal flow and end to end flow in case of loop occurred. The end to end flows are based on dijkstra's algorithm to select a shortest path.

Keywords: SDN, STP, Loop Detection, Directed graph.

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High Performance Computing, Computer Science, Mathematics and Engineering
HPC-ORA-03e

Existence and Approximation of Solutions of Coupled Fractional Order Hybrid Differential Equations

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ABSTRACT

Fractional order differential equations are generalization of a class of ordinary differential equations. Recently, the hybrid differential equations have received much attention in mathematical model of biology. In this paper, we study the existence of coupled fractional hybrid differential systems with order $0 < \alpha < 1$ The existence result is proved by constructing a sequence that approximates the coupled solution based on the coupled fixed point theorem of Dhage (2015). We also illustrate the result by numerical computation example.

Keywords: Approximation of solutions, Caputo fractional derivative, Coupled fixed point, Hybrid differential equations,

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Differential equations learning from spatial-time series data by the fast iterative shrinkage thresholding algorithm

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ABSTRACT

The numerical method of data-driven modelling is presented in this work. It can be used to find the corresponding governing equations in the forms of differential equations from some spatial and time series data that are usually collected from measurements or experiments in real situation. We apply the linear sparse regression technique that can be referred to one of the powerful technique in machine learning algorithm. Here we propose to apply the Fast Iterative Shrinkage-Thresholding Algorithm (FISTA) and then study the capability of its predictions. Some practical applications from real data are demonstrated to show the efficiency of our presented method.

Keywords: Data-driven Modelling, Differential Equation, Fast Iterative Shrinkage-Thresholding Algorithm, Governing Equation, Linear Sparse Regression, Machine Learning.

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High Performance Computing, Computer Science, Mathematics and Engineering
HPC-ORA-05e

Wavelet Galerkin Method for solvig Korteweg-de Vries Equation with Neumann Boundary Conditions

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ABSTRACT

The Wavelet Galerkin method with suitable wavelet basis under the multiresolution analysis for solving the Korteweg-de Vries (KdV) equation is presented in this work. In order to improve the accuracy of numerical solution, the wavelet coefficients are increased to the next level after the coefficient in the previous level is known. This forms a nonlinear system corresponding to the wavelet level specified. Then the nonlinear system is solved by the Newton method. The unknown wavelet coefficients at the boundary are also solved in time space. The accuracy of the presented method is demonstrated by various flow problems that described by the KdV model.

Keywords: Korteweg-de Vries Equation, Newton Method, Multiresolution, Wavelet Galerkin

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