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COMPUTATIONAL SCIENCE AND ENGINEERING ASSOCIATION


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Center of Excellence


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GLOBAL
LEADERSHIP
CaRe NETWORK


RERC
Theory & Practice


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SIFT


Hewlett Packard
Enterprise


TONI
TECH

Welcome Message:

Dr. Supawadee Namuangruk

President of Computational Science and Engineering Association (CSEA), Thailand

E-mail: supawadee@nanotec.or.th

Dear Colleagues,

It is a great honor to extend a warm invitation for you to attend the ANSCSE26, the 26th International Annual Symposium on Computational Science and Engineering, to be held on July 20-22, 2023. This year the symposium is organized by the Faculty of Science, King Mongkut's University of Technology Thonburi (KMUTT), Computational Science and Engineering Association (CSEA), and National Nanotechnology Center (NANOTEC). ANSCSE has always been one of the greatest gatherings of computational science and engineering researchers. After 26 years, we have seen many signs of progress and many exciting research being conducted in this area and the vital role of computational science in real social problems becomes clearer and clearer day by day.

One of the great spirits of ANSCSE is the live discussion among fellow international researchers on the advancement in all fields of computational science and engineering. After a few days of intense discussion on our research, the organizers kindly arranged an excursion to Nong Nooch Tropical Garden & Cultural Village, Pattaya. Finally, thank you in advance for sharing your research, thoughts, and ideas in ANSCSE26 and I look forward to meeting all of you.

Best wishes,

Dr. Supawadee Namuangruk

President of Computational Science and Engineering Association (CSEA), Thailand

Welcome Message:

Prof. Dr. Poom Kumam

ANSCSE 26 Chairman

E-mail: poom.kum@kmutt.ac.th

It is such a great honor for KMUTT to be hosting the 26th ANSCSE this year. We are very pleased that the events of such an exciting field of science are brought to our university. As computational method becomes increasingly more important in Science and Engineering, the need to collaborate and exchange ideas and experiences become more important as well. ANSCSE has a long history of being the major forum for computational scientists to communicate their ideas to their fellow scientists. Recently, the use of computational techniques has been extended to a broader domain of problems beyond science, such as the attempt to understand economy, human society, social networking. Especially, computational techniques are also utilized to hit global problems and goals, such as, renewable energy and pollutions, which leads the thematic area of this version of ANSCSE as the 'Modern Computational Approaches for Decarbonized Society'. This year, we return to have our first full onsite conference since the COVID-19 pandemic, with many interesting international keynote speakers, workshops, and also presentations by many exciting researchers. I am confident that with the experience of the organizing team from KMUTT and strong academic committees from CSEA, we will have a great and fruitful conference. Finally, thank you for coming and we look forward to seeing all the participants in Pattaya.

Best wishes,

Prof. Dr. Poom Kumam

ANSCSE 26 Chairman

Center of Excellence in Theoretical and Computational Science (TaCS-CoE),
Faculty of Science, King Mongkut's University of Technology Thonburi (KMUTT), Thailand.

CSEA Pioneer Award 2023:

Prof. Dr. Supot Hannongbua

ANSCSE 26 Chairman

E-mail: poom.kum@kmutt.ac.th

Professor Dr. Supot HANNONGBUA is a renowned computational chemist and materials scientist in Thailand. He earned his Ph.D. in Computational Chemistry from Innsbruck University in Austria in 1985. Currently a Professor at the Department of Chemistry, Faculty of Science in Chulalongkorn University, he has made significant contributions to the field.

Dr. Supot's academic career is complemented by his administrative roles. He served as the President of the Science Society of Thailand under the Patronage of his Majesty the King, the Director of the Metallurgy and Material Science Research Institute and the Dean of the Faculty of Science at Chulalongkorn University. He is also a member of various boards, including the Office of the Education Council in Thailand, the National Metal and Materials Technology Center (MTEC), the National Science Museum of Thailand, and the Institute for the Promotion of Teaching Science and Technology (IPST). Currently as a member of the National Research and Innovation Committee, Supot actively contributes to shaping the research landscape and fostering innovation in the country.

Dr. Supot's exceptional work has earned him numerous accolades. He has been recognized with the Young Scientist Award, the TWAS Prize for Young Scientists in Thailand, the National Award for the Distinguished Researcher in the Field of Physical Science and Mathematics, and the Outstanding Scientist. He has also received the TRF Senior Scholarship and the Most Cited TRF-Research Publication Award. In addition, he has been honored as an Outstanding Alumnus by KhonKaen University and the Faculty of S cience at Mahidol University. With over 205 publications in international journals, Supot's research has had a global influence. His expertise in computational chemistry and materials science has expanded our understanding of these fields.

Beyond his academic pursuits, he is the founder of two successful startups, Siam Snail Company Ltd. and Unique Natural Company Ltd., which explore innovative and sustainable solutions based on fundamental scientific research. With a remarkable blend of academic excellence, leadership skills, entrepreneurial acumen, and a passion for scientific discovery, Professor Dr. Supot HANNONGBUA continues to be an influential figure in the scientific community. His contributions to research, education, and innovation have left an indelible mark on the scientific landscape, inspiring countless individuals to pursue excellence and explore the mysteries of the natural world.

ANSCSE26 Chair and Co-Chair:

Poom Kumam (Chair)	TaCS-CoE, King Mongkut's University of Technology Thonburi (KMUTT), Thailand
Thana Sutthibutpong (Co-Chair)	King Mongkut's University of Technology Thonburi (KMUTT), Thailand

Steering Committees

Vudhichai Parasuk	Chulalongkorn University, Thailand
Supa Hannongbua	Kasetsart University, Thailand
Supawadee Namuangruk	NSTDA, Thailand

International Scientific Committees/Invited Speakers

Nicu Sebe	University of Trento, Italy
Enrique Zuazua	Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Thorsten Dickhaus	University of Bremen, German
Yoel Je Cho	Gyeongsang National University, South Korea
Ovidiu Bagdasar	University of Derby, United Kingdom
Yasuteru Shigeta	University of Tsukuba, Japan
Deva Priyakumar	International Institute of Information Technology, India
Daniel Escudero	KU Leuven, Belgium
Momoji Kubo	Institute for Materials Research, Tohoku University, Japan
Akira Nakayama	The University of Tokyo, Japan
Norio Yoshida	Nagoya University, Japan
Hisashi Okumura	Institute for Molecular Science, Japan
Ryuhei Harada	University of Tsukuba, Japan
Vannajan Sanghiran Lee	University of Malaya, Malaysia
Antonio Liotta	University of Bozen-Bolzano, Italy
Talha Anwar	King Mongkut's University of Technology Thonburi, Thailand
Cathal Gurrin	Dublin City University, Ireland
Piyabut Burikam	Chulalongkorn University, Thailand
Ninnat Dangniam	The Institute for Fundamental Study, Thailand
Areeya Chantasri	Mahidol University, Thailand
Adisak Boonchun	Kasetsart University, Thailand
Annop Ektarawong	Kasetsart University, Thailand
Manaswee Suttipong	Chulalongkorn University, Thailand
Nuttapon Yodsin	Silpakorn University, Thailand
Anchalee Junkaew	NSTDA, Thailand

Jirasak Wong-ekkabut	Kasetsart University, Thailand
Charin Modchang	Mahidol University, Thailand
Treenut Saithong	King Mongkut's University of Technology Thonburi, Thailand
Teeraphan Laomettachit	King Mongkut's University of Technology Thonburi, Thailand
Panupong Mahalapbutr	Khon Kaen University, Thailand
Yuttasart Nitipaichit	National Telecom Public Company Limited, Thailand
Suthep Suantai	Chiang Mai University, Thailand
Booncharoen Sirinaovakul	King Mongkut's University of Technology Thonburi, Thailand
Supavadee Aramvith	Chulalongkorn University, Thailand

Scientific Chair Sessions

Session – MST: *Mathematics and Statistics*

Narin Petrot	Naresuan University, Thailand
Wiyada Kumam	Rajamangala University of Technology Thanyaburi, Thailand
Parin Chaipunya	King Mongkut's University of Technology Thonburi, Thailand

Session – PHQ: *Computational Physics and Quantum Information Science*

Tanapat Deesuwan	King Mongkut's University of Technology Thonburi, Thailand
Sikarin Yoo-Kong	The Institute for Fundamental Study, Thailand
Pakpoom Reunchan	Kasetsart University, Thailand

Session – CHE: *Computational Chemistry, Materials, and Nanotechnology*

Siriporn Jungsuttiwong	Ubon Ratchathani University, Thailand
Nawee Kungwan	Chiang Mai University, Thailand

Session – BIO: *Computational Biology, Bioinformatics, Biochemistry, and Biophysics*

Thanyada Rungrotmongkol	Chulalongkorn University, Thailand
Rungtiva Palangsuntikul	King Mongkut's University of Technology Thonburi, Thailand
Theerapong Puangmali	Khon Kaen University, Thailand

Session – HPC: *High Performance Computing, Computer Science, and Computer Engineering*

Supakit Prueksaaroon	Thammasat University, Thailand
Rardchawadee Silapunt	King Mongkut's University of Technology Thonburi, Thailand
Phond Phunchongharn	King Mongkut's University of Technology Thonburi, Thailand

Session – AIS: *Artificial Intelligence for Science and Engineering*

Rabian Wangkeeree	Naresuan University, Thailand
Nirattaya Khamsemanan	Sirindhorn International Institute of Technology, Thailand
Cholwich Nattee	Sirindhorn International Institute of Technology, Thailand

Session – CFD: *Computational Fluid Dynamics*

Nopparat Pochai	King Mongkut's Institute of Technology Ladkrabang, Thailand
Usa Humphries	King Mongkut's University of Technology Thonburi, Thailand

Session – IEEE: *Computational Engineering and Image Processing*

Phatiphat Thounthong	King Mongkut's University of Technology North Bangkok, Thailand
Thittaporn Ganokratanaa	King Mongkut's University of Technology Thonburi, Thailand

Workshop: *Applications of Network Theory on Computational Biology and Biochemistry*

Thana Sutthibutpong	King Mongkut's University of Technology Thonburi, Thailand
Teeraphan Laomettachit	King Mongkut's University of Technology Thonburi, Thailand
Teerasit Termsaithong	King Mongkut's University of Technology Thonburi, Thailand

TaCS-CoE Meeting and Workshop TRF (IEEE & Engineering)

Parin Chaipunya	King Mongkut's University of Technology Thonburi, Thailand
Songpon Sriwongsa	King Mongkut's University of Technology Thonburi, Thailand
Phatiphat Thounthong	King Mongkut's University of Technology North Bangkok, Thailand

OVERALL PROGRAM

Sessions	
MST	Mathematics and Statistics
PHQ	Computational Physics and Quantum Information Science
CHE	Computational Chemistry, Materials, and Nanotechnology
BIO	Computational Biology, Bioinformatics, Biochemistry, and Biophysics
HPC	High Performance Computing, Computer Science, and Computer Engineering
AIS	Artificial Intelligence for Science and Engineering
CFD	Computational Fluid Dynamics, Solid Mechanics, Atmospheric, and Oceanic
IEE	(IEEE Special Session) Computational Engineering and Image Processing
Workshop	Applications of Network Theory on Computational Biology and Biochemistry

20th July, 2023

Time	Activities				
7:30-9:00	Registration				
9:00-9:50	Opening Ceremony				
9:50-10.30	**Plenary Lecture 1 - "CROSS-MODAL UNDERSTANDING AND GENERATION OF MULTIMODAL CONTENT"** **Prof. Nicu Sebe** - *University of Trento, Italy*				
10:30-10:45	Break				
Time	**Room1**	**Room2**	**Room3**	**Room4**	**Room5**
10:45-11:00	**PHQ-I1**	**BIO-I1**	**CHE-I1**	**MST-I1**	**AIS-I1**
11:00-11:15					
11:15-11:30	**PHQ-I2**	**BIO-I2**	CHE-O1	MST-O1	AIS-O1
11:30-11:45			CHE-O2	MST-O3	AIS-O2
11:45-12:00	PHQ-O1	BIO-O1	CHE-O3	MST-O4	AIS-O3
12:00-12:15	PHQ-O2				
12:15-13:00	Lunch Break				
13:00-13:15	**PHQ-I3**	**BIO-I3**	**CHE-I2**	**MST-I2**	**AIS-I2**
13.15:13.30					
13:30-13:45	**PHQ-I4**	**BIO-I4**		MST-O5	AIS-O4
13:45-14:00			**CHE-I3**	MST-O6	AIS-O5
14:00-14:15	PHQ-O3	BIO-O2	CHE-O4	MST-O7	AIS-O6
14:15-14:30	PHQ-O4		CHE-O5		AIS-O7
14:30-14:45	Break				
14:45-15:00	**CFD-I1**	**BIO-I5**	**CHE-I4**	**MST-I3**	CSEA meeting
15:00-15:15					CSEA meeting
15:15-15:30	PHQ-O5	**BIO-I6**	CHE-O6	MST-O8	CSEA meeting
15:30-15:45	PHQ-O6		CHE-O7	MST-O9	CSEA meeting
15:45-16:00	CFD-O1	BIO-O3	CHE-O8	MST-O10	CSEA meeting
16:00-16:15	CFD-O2	Poster Session			CSEA meeting
16:15-16:30	CFD-O3	Poster Session			CSEA meeting
16:30-18:00	Poster Session				CSEA meeting
18:00-20:00	Welcome Dinner				

21st July, 2023

Time	Activities				
09:00-09:35	**Plenary Lecture 2 - "CONTROL AND MACHINE LEARNING"** **Prof. Enrique Zuazua** - *Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU). Erlangen, Germany*				
09:30-09:55	**Special Lecture - "TOP 7 PREDICTIONS FOR THE FUTURE OF HPC & AI "** **Raj Chhabra** - *Hewlett Packard Enterprise*				
09:55-10:00	Break				
Time	**Room1**	**Room2**	**Room3**	**Room4**	**Room5**
10:00-10:15	**HPC-I1**	**BIO-I7**	**CHE-I5**	**MST-I4**	**IEEE-I1**
10:15-10:30					
10:30-10:45	**HPC-I2**	**BIO-I8**	**CHE-I6**	MST-O11	**IEEE-I2**
10:45-11:00				MST-O12	
11:00-11:15	HPC-O1	BIO-O4	**CHE-I7**	MST-O13	IEEE-O1
11:15-11:30	HPC-O2	BIO-O5		MST-O14	IEEE-O2
11:30-11:45	HPC-O3		CHE-O9	MST-O15	IEEE-O3
11:45-12:00	HPC-O4		CHE-O10		IEEE-O4
12:00-12:15	HPC-O5		CHE-O11		
12:15-13:00	Lunch Break				
13:00-13:15	**HPC-I3**	**BIO-I9**	**CHE-I8**	**MST-I5**	**IEEE-I3**
13.15:13.30					
13:30-13:45	HPC-O6	**BIO-I10**	**CHE-I9**	MST-O16	IEEE-O5
13:45-14:00	HPC-O7			MST-O17	IEEE-O6
14:00-14:15	HPC-O8	BIO-O6	CHE-O12	MST-O18	IEEE-O7
14:15-14:30	HPC-O9	BIO-O7	CHE-O13	MST-O19	IEEE-O8
14:30-14:45	HPC-O10		CHE-O14	MST-O20	IEEE-O9
14:45-15:00	HPC-O11	Break			
15:00-15:15	workshop			TaCS Meeting	**IEEE-I4**
15:15-15:30	workshop			TaCS Meeting	
15:30-15:45	workshop			TaCS Meeting	**IEEE-I5**
15:45-16:00	workshop			TaCS Meeting	
16:00-16:15	workshop			TaCS Meeting	IEEE-O10
16:15-16:30	workshop			TaCS Meeting	IEEE-O11
16:30-16:45	workshop			TaCS Meeting	IEEE-O12
16:45-17:00	workshop			TaCS Meeting	IEEE-O13
17:00-17:15	Break				
17:15-17:45	Closing Ceremony				

22nd July, 2023

Time	Activities
09:00-14:30	**Excursion Activity** *Nongnooch Tropical Garden, Pattaya, Chonburi.*

PHQ	Computational Physics and Quantum Information Science
CFD	Computational Fluid Dynamics

20th July, 2023 Supannahong Room

Morning Session: Chairs - Asst.Prof.Dr. Sikarin Yoo-Kong, Dr.Tanapat Deesuwan

Time	Code	Topics	Speakers
10:45-11:00	**PHQ-I1**	**IMAGINARY TIME AND TEMPERATURE**	Prof. Dr. Piyabut Burikam
11:00-11:15			*Chulalongkorn University, Thailand*
11:15-11:30	**PHQ-I2**	**QUANTUM SAMPLING ADVANTAGE: HOW TO PROVE IT AND DOES IT MATTER?**	Dr. Ninnat Dangniam
11:30-11:45			*IF*
11:45-12:00	PHQ-O1	NUMERICAL RELATIVITY SIMULATION OF BINARY BLACK HOLE MERGER	Assoc.Prof.Dr. Teparksorn Pengpan

20th July, 2023 Supannahong Room

Afternoon Session: Chairs - Assoc.Prof.Dr.Pakpoom Reunchan, Assoc.Prof.Dr.Thana Sutthibutpong

Time	Code	Topics	Speakers
13:00-13:15	**PHQ-I3**	**COMBINING MLFF WITH DFT: EXAMPLES OF MXENES AND TMDS**	Assoc.Prof.Dr. Adisak Boonchun
13.15:13.30			*KU*
13:30-13:45	**PHQ-I4**	**ATOMIC-SCALE DESIGN OF METAL-DIBORIDE THIN FILM-BASED HARD COATING TECHNOLOGY**	Assoc.Prof.Dr. Annop Ektarawong
13:45-14:00			*CU*
14:00-14:15	PHQ-O3	ACCURACY OF COARSE-GRAINED MARTINI MODEL IN PREDICTING NANOPARTICLE DIFFUSION COEFFICIENTS: A COMPARATIVE STUDY FOR OLEIC-MAGNETITE NANOPARTICLES	Mr.Nopparuj Sodsri
14:15-14:30	PHQ-O4	FREQUENCY-DOMAIN INVERSION OF TERAHERTZ INTENSITY DATA USING A HYBRID MODELING METHOD	Mr.Sirawit Inpuak

20th July, 2023 **Supannahong Room**

Evening Session: Chairs - Assoc.Prof.Dr.Usa Humphries, Assoc.Prof.Dr.Nopparat Pochai

Time	Code	Topics	Speakers
14:45-15:00 15:00-15:15	**CFD-I1**	**PROPERTIES AND APPLICATIONS OF NANOFLUIDS; THEORY AND MATHEMATICAL MODELING**	Dr.Talha Anwar *KMUTT*
15:15-15:30	PHQ-O5	SIMULATION OF PLASMA OPERATION WITH SMBI FUELING IN OHMIC MODE FOR THE THAILAND TOKAMAK-1 USING THE TASK/TR INTEGRATED MODELING CODE	Mr.Kitti Rongpuit
15:30-15:45	PHQ-O6	STUDYING THE BEHAVIOR OF CHARGE CARRIERS IN THIN-FILM PEROVSKITE DEVICES UNDER PRE-BIAS SPACE-CHARGE-LIMITED CURRENT MEASUREMENTS BY MEANS OF DRIFT–DIFFUSION SIMULATIONS	Mr.Watcharanon Kantayasakun
15:45-16:00	CFD-O1	KINETICS MODELING OF TRANSPORT PHENOMENA IN CORROSIVE SYSTEM PIPELINE	Ms.Siriwan Pumkathin
16:00-16:15	CFD-O2	SPECTRAL PROPER ORTHOGONAL DECOMPOSITION OF FLOW PAST CIRCULAR CYLINDER AT SUBCRITICAL REYNOLD'S NUMBER WITH SYNTHETIC JET	Mr.Aritouch Puengrung
16:15-16:30	CFD-O3	HEAT TRANSFER ANALYSIS OF ZnO+Al2O3+TiO2/DW BASED TERNARY HYBRID NANOFLUID: A FRACTAL-FRACTIONAL MODEL	Mr.Saqib Murtaza

AIS Artificial Intelligence for Science and Engineering

20th July, 2023 **Ratchanawee 2 Room**

Morning Session: Chairs - Prof.Dr.Rabian Wangkeeree, Assoc.Prof.Dr.Nirattaya Khamsemanan

Time	Code	Topics	Speakers
10:45-11:00 11:00-11:15	**AIS-I1**	**CONCURRENT SENSING AND LEARNING WITH IN-NODE MACHINE LEARNING**	Prof. Antonio Liotta *University of Bozen-Bolzano, Italy*
11:15-11:30	AIS-O1	STREAMFLOW FORECASTING BY ARTIFICIAL NEURAL NETWORKS IN DIFFERENT CLIMATIC ZONES	Mr.Muhammad Waqas
11:30-11:45	AIS-O2	LAND USE AND LAND COVER PREDICTIONS WITH QGIS-BASED MACHINE LEARNING ALGORITHMS: A CASE STUDY OF THA CHIN RIVER BASIN, THAILAND	Mr.Phyo Thandar Hlaing
11:45-12:00	AIS-O3	MACHINE LEARNING-BASED COMMUNICATION POWER ADAPTATION FOR CONNECTED TRUCK PLATOONING	Mr.Sirapob Keeratichandecha

20th July, 2023 **Ratchanawee 2 Room**

Afternoon Session: Chairs - Prof.Dr.Rabian Wangkeeree, Assoc.Prof.Cholwich Nattee

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**AIS-I2**	**EXPLORING PROBLEM SOLVING AND OPTIMIZATION: HEURISTIC, META-HEURISTIC AND HYPER-HEURISTIC SEARCH METHODS**	Prof. Booncharoen Sirinaovakul *Computer Engineering, Faculty of Engineering, King Monkut's University of Technology Thonburi (KMUTT)*
13:30-13:45	AIS-O4	CLASSIFICATION OF SENTINEL-2 IMAGES FOR THAILAND'S PLANTATION DETECTION	Mr.Wongnaret Khantuwan
13:45-14:00	AIS-O5	DEEP LEARNING FOR COCONUT TREE DECTECTING WITH SATELLITE IMAGERY	Mr.Chaiyasit Tanchotsrinon
14:00-14:15	AIS-O6	ONLINE SOC AND SOH ESTIMATION OF LI-ION BATTERY IN ELECTRIC VEHICLES: ARTIFICIAL NEURAL NETWORK	Mr.Nutthanin Choongam
14:15-14:30	AIS-O7	A PHYSICS-INFORMED NEURAL NETWORK FOR THE DRIFT-DIFFUSION MODEL'S SOLUTIONS TO STUDY SPACE-CHARGE-LIMITED CURRENT DENSITIES IN MILLIMETER-THICK MAPbBr3 PEROVSKITE WITH ION MIGRATION	Mr.SHUAIBU SANI

HPC High Performance Computing, Computer Science, and Computer Engineering

21st July, 2023 **Supannahong Room**

Morning Session: Chairs - Asst.Prof.Dr.Phond Phunchongharn, Assoc.Prof.Dr.Rardchawadee Silapunt

Time	Code	Topics	Speakers
10:00-10:15 10:15-10:30	**HPC-I1**	**THE DEVELOPMENT OF GOVERNMENT DIGITAL INFRASTRUCTURE WITH THE NEED OF HIGH PERFORMANCE COMPUTING SYSTEMS**	Dr. Yuttasart Nitipaichit *National Telecom Public Company Limited*
10:30-10:45 10:45-11:00	**HPC-I2**	**DATA-CENTRIC ACCELERATOR DESIGNS FOR HPC WORKLOADS**	Asst. Prof. Dr. Rachata Ausavarungnirun *The Sirindhorn International Thai-German Graduate School of Engineering, King Mongkut's University of Technology North Bangkok*
11:00-11:15	HPC-O1	BLOCKCHAIN TECHNOLOGY TO ENHANCE SUPPLY CHAIN MANAGEMENT: CASE STUDY OF COVID-19 ANTIGEN TEST KIT	Mr. Raned Chuphueak
11:15-11:30	HPC-O2	BLOCKCHAIN TECHNOLOGY FOR HEALTHCARE NETWORKS	Mr.Sorawid Juntachat
11:30-11:45	HPC-O3	Cost-Sensitive Cloud Architecture for an Online Assessment Web Application	Mr.Subtawee Hanyut
11:45-12:00	HPC-O4	AGRICULTURAL DATA SHARING TO APPLICATIONS VIA THAGRI	Ms.Jutarat Khiripet
12:00-12:15	HPC-O5	DESIGN AND DEVELOPMENT OF THE BACK-END SYSTEM FOR AN ONLINE LEARNING ASSESSMENT PLATFORM	Mr.Watcha Sasawattakul

21st July, 2023 **Supannahong Room**

Afternoon Session: Chairs - Asst.Prof.Dr.Phond Phunchongharn, Asst.Prof.Dr.Supakit Prueksaaroon

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**HPC-I3**	**DOES HPC MATTER? REFLECTIONS ON THE UTILITY OF SUPERCOMPUTING**	Prof. Dr. Sally Goldin *Carnegie-Mellon University Thailand*
13:30-13:45	HPC-O6	A DIVISION ALGORITHM ON MATULA NUMBER SYSTEM	Ms.Nattanan Watcharakasemsin
13:45-14:00	HPC-O7	INDIRECT SLIDING MODE CONTROL APPLIED TO FAST BATTERY CHARGER OF LIGHT ELECTRIC VEHICLES	Mr.Songklod Sriprang
14:00-14:15	HPC-O8	MODEL AND SIMULATION CURRENT CONTROL OF LED STREET LING BASED ON IBFC CONVERTER OPERATE IN STANDBY MODE	Mr.Thananchai Jinati
14:15-14:30	HPC-O9	SUGARCANE YIELD PREDICTION BASED ON SATELLITE INDICES AND CLIMATE DATA IN THAILAND	Ms.Pornpimon Sinpayak
14:30-14:45	HPC-O10	HYPERMAP GRAMMAR FOR PLANAR K-TREE MAPS	Mr.Worawut Komekarat
14:45-15:00	HPC-O11	A COMPARISON OF QUANTUM GRADIENTS	Mr.Natchapol Patamawisut

IEE (IEEE Special Session) Computational Engineering and Image Processing

21st July, 2023 **Ratchanawee 2 Room**

Morning Session: Chairs - Prof. Dr.Phatiphat Thounthong, Dr. Thittaporn Ganokratanaa

Time	Code	Topics	Speakers
10:00-10:15 10:15-10:30	**IEEE-I1**	**MULTIMODAL USER MODELS FOR LIFE ENHANCEMENT**	Assoc. Prof. Dr. Cathal Gurrin *School of Computing, Dublin City University, Ireland*
10:30-10:45 10:45-11:00	**IEEE-I2**	**CAUSALITY INSPIRED RETRIEVAL OF HUMAN-OBJECT INTERACTIONS FROM VIDEO**	Asst. Prof. Dr. Liting Zhou *School of Computing, Dublin City University, Ireland*
11:00-11:15	IEEE-O1	OPTIMIZATION OF MUTUAL INDUCTANCE COIL DESIGN FOR WIRELESS POWER TRANSFER USING MATLAB/SIMULINK	Assoc.Prof.Dr.Worapong Pairindra
11:15-11:30	IEEE-O2	INVESTIGATION AUTOMATE ALGORITHM FOR FINDING FOCUS AND EXPOSURE OF QUALITY CONTROL SYSTEM IN INDUSTRY	Mr.Rapeephat Yodsungnoen
11:30-11:45	IEEE-O3	A GENERALIZED LIU-STOREY SPECTRAL CONJUGATE GRADIENT METHOD WITH APPLICATIONS IN ROBOT CONTROL AND IMAGE RESTORATION MODELS	Nasiru Salihu
11:45-12:00	IEEE-O4	IMPROVED NEH ALGORITHM FOR PERMUTAION FLOWSHOP SCHEDULING	Mr.RUNGROT PHOLYIAM

21st July, 2023 **Ratchanawee 2 Room**

Afternoon Session: Chairs - Prof. Dr.Phatiphat Thounthong, Dr. Thittaporn Ganokratanaa

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**IEEE-I3**	**EV AND ENERGY MODERNIZATION PLATFORMS**	Mr. Worapoj Ruenrerngwong *Chosen Group*
13:30-13:45	IEEE-O5	DIFFERENTIAL FLATNESS BASED CONTROL LAW FOR 3-PHASE AC/DC CONVERTER FOR HIGH POWER APPLICATION	Assoc.Prof.Dr.Nitchamon Poonnoy
13:45-14:00	IEEE-O6	EXTENDED HAMILTONIAN CONTROL LAW OF MULTIPHASE BOOST CONVERTER FOR FUEL CELL POWER SOURCE IN DC-MICROGRID APPLICATION	Dr.Burin Yodwong
14:00-14:15	IEEE-O7	DESIGN AND MODELING OF A HAMILTONIAN CONTROL LAW FOR A BIDIRECTIONAL CONVERTER IN DC DISTRIBUTION APPLICATIONS	Mr.Methawin Jantra
14:15-14:30	IEEE-O8	HAMILTONIAN CONTROL LAW APPLICATION FOR A BOOST POWER FACTOR CORRECTION CONVERTER	Mr.Wuttikai Tammawan
14:30-14:45	IEEE-O9	HAMILTONIAN CONTROL LAW APPLICATION FOR CONSTANT CURRENT – CONSTANT VOLTAGE WIRELESS BATTERY CHARGING USING A PRIMARY SIDE BUCK CONVERTER	Mr.Thanet Sriprom

21st July, 2023 **Ratchanawee 2 Room**

Evening Session: Chairs - Prof. Dr.Phatiphat Thounthong, Dr. Thittaporn Ganokratanaa

Time	Code	Topics	Speakers
15:00-15:15 15:15-15:30	**IEEE-I4**	**ARTIFICIAL INTELLIGENCE, -TESTING, AI IN EDUCATION**	Asst.Prof. Dr. Pokpong Songmuang *Faculty of Science and Technology* *Thammasat University*
15:30-15:45 15:45-16:00	**IEEE-I5**	**Predictive Model for Assessing Lithium-Ion Battery Health in Electric Vehicles**	Prof.Dr. Surin Khomfoi *KMITL*
16:00-16:15	IEEE-O10	A PORT- CONTROLLED HAMILTONIAN APPROCH BASED ON SPEED/TORQUE CONTROL FOR PERMANENT MAGNET SYNCHRONOUS MOTOR DRIVES	Mr.Thong-In Suyata
16:15-16:30	IEEE-O11	NON-ISOLATED ONBOARD EV CHARGER CONTROLLER DESIGN BASED ON ADAPTIVE HAMILTONIAN CONTROL LAW	Nattapon Somboonpanya
16:30-16:45	IEEE-O12	MODELLING AND SIMULATION OF PS-MODULATED RESONANT INVERTER BASED ON HAMILTONIAN CONTROL LAW FOR INDUCTION HEATING APPLICATIONS	Mr.Teeruch Janjongcam
16:45-17:00	IEEE-O13	HAMILTONIAN CONTROL LAW FOR FUEL CELL/SUPERCAPACITOR HYBRID SOURCE TO SOLVE CONSTANT POWER LOAD STABILITY ISSUES IN DC MICROGRID	PONGSIRI MUNGPORN

BIO Computational Biology, Bioinformatics, Biochemistry, and Biophysics

20th July, 2023 **Punnarai 1 Room**

Morning Session: Chairs - Assoc.Prof. Rungtiva Poo-Aporn, Assoc.Prof. Theerapong Puangmali

Time	Code	Topics	Speakers
10:45-11:00 11:00-11:15	**BIO-I1**	**DEVELOPMENT OF MOLECULAR THEORY OF SOLVATION FOR BIOMOLECULAR SYSTEMS**	Prof. Norio Yoshida *Nagoya University, Japan*
11:15-11:30 11:30-11:45	**BIO-I2**	**AGGREGATION AND DISAGGREGATION OF AMYLOID-β PEPTIDES OBSERVED BY ALL-ATOMS MOLECULAR DYNAMICS SIMULATIONS**	Assoc. Prof. Hisashi Okumura *Institute for Molecular Science, Japan*
11:45-12:00	BIO-O1	In Silico Studies of Selected Metformin Derivatives Against α-glucosidase and α-amylase as potential antidiabetic drug.	Ms. Nor Akmalyati Sulong

20th July, 2023 **Punnarai 1 Room**

Afternoon Session: Chairs - Assoc.Prof. Rungtiva Poo-Aporn, Prof. Norio Yoshida

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**BIO-I3**	**COMPUTATIONAL PROTEIN DESIGN: DRIVING INNOVATION THROUGH DYNAMICS AND ENERGY OPTIMIZATION**	Assoc. Prof. Dr. Vannajan Sanghiran Lee *University of Malaya*
13:30-13:45 13:45-14:00	**BIO-I4**	**EXPLORING THE MOLECULAR MECHANISMS OF GRAPHENE QUANTUM DOT-BASED DIABETES APTASENSOR TO DETECT GLYCATED HUMAN SERUM ALBUMIN IN A SOLUTION**	Assoc. Prof. Dr. Prapasiri Pongprayoon *Kasetsart University*
14:00-14:15	BIO-O2	Cyclicpeptifinder: a deep learning approach for cyclic peptide drug discovery through ligand prediction	Mr.Duan Lian

20th July, 2023 **Punnarai 1 Room**

Evening Session: Chairs - Assoc.Prof. Theerapong Puangmali, Assoc. Prof. Dr. Vannajan Sanghiran Lee

Time	Code	Topics	Speakers
14:45-15:00 15:00-15:15	**BIO-I5**	**FROM NUMBERS TO INSIGHTS: HOW MATHEMATICS EMPOWERS DISEASE SURVEILLANCE AND PREDICTION**	Assoc. Prof. Charin Modchang *Mahidol University*
15:15-15:30 15:30-15:45	**BIO-I6**	**OMICS DATA ANALYTIC AND MODELING TO SIMULATE A JOURNEY OF CARBON CONVERSION TOWARDS PLANT BIOMASS PRODUCTION**	Assoc. Prof. Dr. Treenut Saithong *King Mongkut's University of Technology Thonburi*
15:45-16:00	BIO-O3	Wavelet analysis of influenza epidemics associated with pm10 and meteorological factors in bangkok, thailand	Dr.Suparinthon Anupong

21st July, 2023 **Punnarai 1 Room**

Morning Session: Chairs - Assoc.Prof. Thanyada Rungrotmongkol, Asst. Prof. Dr. Panupong Mahalapbutr

Time	Code	Topics	Speakers
10:00-10:15 10:15-10:30	**BIO-I7**	**PARALLEL CASCADE SELECTION MOLECULAR DYNAMICS FOR SAMPLING RARE EVENTS OF PROTEINS**	Assoc. Prof. Ryuhei Harada *University of Tsukuba, Japan*
10:30-10:45 10:45-11:00	**BIO-I8**	**AGGREGATION OF FULLERENES IN BIOLOGICAL MEMBRENE: MOLECULAR DYNAMICS SIMULATIONS**	Assoc.Prof. Jirasak Wong-ekkabut *Kasetsart University*
11:00-11:15	BIO-O4	Improving solubility and stability of piperine using beta-cyclodextrin derivatives: A combined computational and experimental study	Ms. Saba Ali
11:15-11:30	BIO-O5	Screening for plant regulators modulating the early disease-state transition of cassava brown streak disease (cbsd) using dynamic network biomarker (dnb)	Mr.Nattavat Sukko

21st July, 2023 **Punnarai 1 Room**

Afternoon Session: Chairs -Assoc. Prof. Dr. Treenut Saithong, Assoc. Prof. Ryuhei Harada

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**BIO-I9**	**PREDICTION OF CANCER DRUG SYNERGY USING MECHANISTIC MODELING AND DEEP LEARNING**	Asst. Prof. Teeraphan Laomettachit *King Mongkut's University of Technology Thonburi*
13:30-14:00	**BIO-I10**	**ANILINONAPHTHOQUINONES AS POTENT EGFR INHIBITORS: A COMBINED EXPERIMENTAL AND THEORETICAL STUDY**	Asst. Prof. Dr. Panupong Mahalapbutr *Khon Kaen University*
14:00-14:15	BIO-O6	A compartment model of cannabidiol pharmacokinetics after sublingual administration, and application	Mr.Thanachok Mahahong
14:15-14:30	BIO-O7	Modeling covid-19 transmission in thailand: the role of vaccination, npis, and treatment	Mr.Alhassan Ibrahim

CHE Computational Chemistry, Materials, and Nanotechnology

20th July, 2023 Punnarai 2 Room

Morning Session: Chairs - Assoc.Prof.Dr. Nawee Kungwan, Dr. Wutthikrai Busayaporn

Time	Code	Topics	Speakers
10:45-11:00 11:00-11:15	**CHE-I1**	**TRANSITION METAL CO INTERACTION REVISITED WITH A TWIST OF SPIN**	Dr. Kaito Takahashi *Institute of Atomic and Molecular Sciences Academia Sinica, Taiwan*
11:15-11:30	CHE-O1	EXPLORING THE IMPACT OF Fe DOPING ON THE ELECTROCATALYTIC ACTIVITY OF NIOOH FOR HMF-TO-FDCA OXIDATION: A FIRST-PRINCIPLES APPROACH	Dr.Chattarika Sukpattanacharoen
11:30-11:45	CHE-O2	Theoretical study of the relation between the dressed states and dynamic Stark shift in presence of non-resonant elliptically polarized laser	Dr.Hirobumi Mineo
11:45-12:00	CHE-O3	INVESTIGATING AXIAL LIGAND FUNCTIONALIZED 2D COBALT PORPHYRIN MOFS FOR PHOTOCATALYTIC CO2 REDUCTION: A DFT STUDY	Ms.Jirawattana Rungruengkit

20th July, 2023 Punnarai 2 Room

Afternoon Session: Chairs - Assoc.Prof.Dr. Nawee Kungwan, Dr. Nuttapon Yodsin

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**CHE-I2**	**MOLECULAR/MATERIAL GENERATORS: DE NOVO DESIGN USING MODERN MACHINE LEARNING METHODS**	Prof. Deva Priyakumar *Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, India*
13:30-13:45 13:45-14:00	**CHE-I3**	**MODELLING FLUORESCENCE AND PHOSPHORESCENCE FROM-FIRST-PRINCIPLES**	Prof. Daniel Escudero *KU Leuven, Belgium*
14:00-14:15	CHE-O4	INSIGHTS INTO THE OXYGEN EVOLUTION REACTION MECHANISM ON IRON-COBALT-NIKEL-MOLYBDENUM HIGH-ENTROPY ALLOY CATALYSTS: A COMBINED DENSITY FUNCTIONAL THEORY AND MACHINE LEARNING STUDY	Mr.Panupol Untarabut
14:15-14:30	CHE-O5	MULTI-SCALE SIMULATION APPROACH FOR STRUCTURE OPTIMIZATION OF DYE-SENSITIZED SOLAR CELL DEVICES	Dr.Mari Onodera

20th July, 2023 Punnarai 2 Room

Evening Session: Chairs - Dr. Wutthikrai Busayaporn, Assoc.Prof.Dr. Nawee Kungwan

Time	Code	Topics	Speakers
14:45-15:00 15:00-15:15	**CHE-I4**	**ENHANCING PERFORMANCE OF V2O5 CATHODES IN LI-ION BATTERIES THROUGH FIRST-PRINCIPLES-BASED HETEROSTRUCTURE ENGINEERING AND CONTROLLED DOPING**	Asst. Prof. Dr. Suwit Suthirakun *School of Chemistry, Institute of Science, Suranaree University of Technology, Thailand*
15:15-15:30	CHE-O6	FIRST–PRINCIPLES STUDY OF SURFACE SEGREGATION ON BIMETALIC CuZn(111) IN PRESENCE OF VARIOUS GAS ADSORBED FOR CARBON–DIOXIDE REDUCTION REACTION (CO2RR)	Ms.Arisa Kaewpratum
15:30-15:45	CHE-O7	MERCURY OXIDATION AND METHYLATION REACTIONS IN NATURAL GAS PROCESSING WITH SOLVATION EFFECTS: A DFT STUDY	Mr.Pheerawich Laokulwanich
15:45-16:00	CHE-O8	THE CATALYTIC ACTIVITY OF SINGLE TRANSITION METAL ATOM DECORATED IN NITROGEN-DOPED GRAPHENE FOR HCOOH DEHYDROGENATION: A DFT STUDY	Ms.Pimjai Pimbaotham

21st July, 2023 Punnarai 2 Room

Morning Session: Chairs - Prof. Deva Priyakumar, Dr. Nuttapon Yodsin

Time	Code	Topics	Speakers
10:00-10:15 10:15-10:30	**CHE-I5**	**SUPERCOMPUTER "MASAMUNE-IMR" GIVES PARADIGM SHIFTS ON SOLID OXIDE FUEL CELL SIMULATIONS**	Prof. Momoji Kubo *Institute for Materials Research, Tohoku University, Japan*
10:30-10:45 10:45-11:00	**CHE-I6**	**MICROSCOPIC UNDERSTANDING OF INTERFACE AT LIQUID/SOLID-OXIDE AND MOLECULAR ADSORPTION ON THE SURFACE BY NEURAL NETWORK POTENTIALS**	Prof. Akira Nakayama *Department of Chemical System Engineering, The University of Tokyo*
11:00-11:15 11:15-11:30	**CHE-I7**	**LITHIUM-ION SOLVATION AND TRANSPORT PROPERTIES IN BULK ORGANIC ELECTROLYTES FROM CLASSICAL MOLECULAR DYNAMICS**	Dr. Manaswee Suttipong *Chulalongkorn University*
11:30-11:45	CHE-O9	RELATIONSHIP BETWEEN THE WATER DISTRIBUTION ON CARBON SUPPORT SURFACE AND PROTON CONDUCTION PATH : LARGE-SCALE REACTIVE MOLECULAR DYNAMICS SIMULATIONS	Mr.Tetsuya Nakamura
11:45-12:00	CHE-O10	THE DIFFUSION COEFFIECIENT OF MERCURY AND MERCURY COMPOUNDS IN CRUDE OIL AND WATER AT DIFFERENT POSSIBLE TEMPERATURES	Mr.Tat Tangpirul
12:00-12:15	CHE-O11	A MOLECULAR DYNAMICS SIMULATIONS STUDY OF GALLIUM MONOLAYER AS A SUPERCAPACITOR APPLICATION	Mr.Muhammad Zhafran Zakaria

21st July, 2023 **Punnarai 2 Room**

Afternoon Session: Chairs - Asst. Prof. Dr. Suwit Suthirakun, Dr. Manaswee Suttipong

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**CHE-I8**	**THEORETICAL STUDIES ON THE STRUCTURES AND FUNCTIONS OF METALLOPROTEINS: TOWARDS UNDERSTANDING OF INHIBITION MECHANISMS OF CCO AND HPPD**	Prof. Yasuteru Shigeta *University of Tsukuba, Japan*
13:30-13:45 13:45-14:00	**CHE-I9**	**DISCOVERY OF MO-B EMBEDDED C2N AS A HIGHLY EFFICIENT ELECTROCATALYST FOR UREA PRODUCTION FROM N2 AND CO2 THROUGH HIGH THROUGHPUT**	Dr. Nuttapon Yodsin *Department of Chemistry, Faculty of Science, Silpakorn University, Thailand*
14:00-14:15	CHE-O12	COMPUTATIONAL SCREENING OF TRANSITION METAL DOPED MO2B2O2 AS CATHODE MATERIALS OF LI-SULFUR BATTERIES	Mr.Wongsathorn Kaewraung
14:15-14:30	CHE-O13	CARBON DIOXIDE REDUCTION REACTION ON NON-METAL-DOPED GRAPHITIC CARBON NITRIDE CATALYST: A DFT STUDY	Ms.Wassana Mongkonkan
14:30-14:45	CHE-O14	ENHANCING THE PERFORMANCE AND STABILITY OF PEROVSKITE SOLAR CELLS THROUGH POTASSIUM HALIDE SURFACE TREATMENT AT THE SNO2/PEROVSKITE INTERFACE: A COMBINED EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDY	Mr.IBRAHIM MUHAMMAD ADAM

20th July, 2023 **Ratchanawee 1 Room**

Morning Session: Chairs - Prof.Dr.Poom Kumam, Dr.Parin Chaipunya

Time	Code	Topics	Speakers
10:45-11:00 11:00-11:15	**MST-I1**	**USING MAPLE FOR COMPUTING EXPONENTIAL INTEGRALS OVER POLYTOPES**	**Prof. Dr. Thorsten Dickhaus** ***Institute for Statistics, University of Bremen, German***
11:15-11:30	MST-O1	BILEVEL GAMES WHOSE FOLLWERS ARE FUZZY AND IRRATIONAL	Mr.Yutthakan Chummongkhon
11:30-11:45	MST-O3	LONG-RANGE CORRELATION BEHAVIOR OF RESTING-STATE EEG SIGNAL WITH APPLICATION IN MAJOR DEPRESSIVE DISORDER DIAGNOSIS	Ms.Airin Intaratat
11:45-12:00	MST-O4	PROVINCE SCALE RICE YIELD PREDICTION USING STATISTIC METHOD	Mr.Chanon Boonkangwan

20th July, 2023 **Ratchanawee 1 Room**

Afternoon Session: Chairs - Prof.Dr.Poom Kumam, Dr.Parin Chaipunya

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**MST-I2**	**SOME PROJECTION METHODS WITH LINE-SEARCH RULES FOR NONLINEAR PROBLEMS IN HILBERT SPACES**	**Prof. Dr. Yoel Je Cho** ***Department of Mathematics Education, Gyeongsang National University, Korea***
13:30-13:45	MST-O5	AN INTEGRATED PICKUP AND DELIVERY PROBLEM AND FEEDER VEHICLE ROUTING PROBLEM	Ms.Chinchet Boonmalert
13:45-14:00	MST-O6	IMAGE INPAINTING VIA THE MODIFIED EXEMPLAR-BASED INPAINTING WITH TWO-STAGE STRUCTURE-TENSOR AND IMAGE SPARSE REPRESENTATION	Ms.Petchraporn Yodjai
14:00-14:15	MST-O7	A MIXED-INTEGER LINEAR PROGRAMMING MODEL FOR SOLVING A MULTI-DEPOT INVENTORY ROUTING PROBLEM WITH PERISHABLE PRODUCTS	Ms.Kevalin Yeesan

20th July, 2023 **Ratchanawee 1 Room**

Evening Session: Chairs - Prof.Dr.Poom Kumam, Dr.Parin Chaipunya

Time	Code	Topics	Speakers
14:45-15:00 15:00-15:15	**MST-I3**	**KEY RESULTS AND RECENT ADVANCES IN DYNAMIC GEOMETRY**	Assoc. Prof. Ovidiu Bagdasar *University of Derby, UK*
15:15-15:30	MST-O8	EKELAND'S VARIATIONAL PRINCIPLE ON NON-TRIANGULAR METRIC SPACES	Ms.Natthaya Boonyam
15:30-15:45	MST-O9	A CONJUGATE GRADIENT METHOD WITH NON-MONOTONE-BASED LINE SEARCH FOR LARGE-SCALE PROBLEMS WITH APPLICATION TO NON-NEGATIVE MATRIX FACTORIZATION PROBLEMS	Mr.Mahmoud Muhammad Yahaya
15:45-16:00	MST-O10	MODIFIED CONJUGATE GRADIENT METHODS FOR VECTOR OPTIMIZATION	Mr.Jamilu Yahaya

21st July, 2023 **Ratchanawee 1 Room**

Morning Session: Chairs - Assoc.Prof.Dr.Wiyada Kumam, Dr.Parin Chaipunya

Time	Code	Topics	Speakers
10:00-10:15 10:15-10:30	**MST-I4**	**STRONG CONVERGENCE OF ALTERNATED INERTIAL CQ RELAXED METHOD WITH APPLICATION IN SIGNAL RECOVERY**	Jamilu Abubakar *KMUTT*
10:30-10:45	MST-O11	CONVERGENCE RESULTS ON A NEW CLASS OF MULTI-VALUED GENERALIZED NONEXPANSIVE MAPPINGS IN BANACH SPACES	Asst.Prof.Dr.Nazli Kadioglu Karaca
10:45-11:00	MST-O12	Inertial CQ-algorithms for k-strict pseudo-contractive mappings in Hilbert Spaces	Asst.Prof.Dr.Solomon Gebregiorgis Teweldemedin
11:00-11:15	MST-O13	A HYBRID METHOD FOR GENERALIZED MIXED EQUILIBRIUM PROBLEMS, ZERO PROBLEMS AND FIXED POINTS OF ASYMPTOTICALLY DEMICONTRACTIVE MAPPINGS IN THE INTERMEDIATE SENSE	Mr.Ahmad Abdulwahab
11:15-11:30	MST-O14	AN EXISTENCE OF MULTI-CRITERIA NASH EQUILIBRIUM BASED ON VECTORIAL RATIONALITY FUNCTION	Ms.Urairat Deepan
11:30-11:45	MST-O15	NEW NORMAL OPERATOR AND ITS PROPERTIES ON CAT(0) SPACES	Ms.Wiparat Worapitpong

21st July, 2023 **Ratchanawee 1 Room**

Afternoon Session: Chairs - Assoc.Prof.Dr.Wiyada Kumam, Dr.Parin Chaipunya

Time	Code	Topics	Speakers
13:00-13:15 13.15:13.30	**MST-I5**	**AN OUTER QUADRATIC APPROXIMATION METHOD FOR SOLVING SPLIT FEASIBILITY PROBLEMS**	Guash Haile Taddele *KMUTT*
13:30-13:45	MST-O16	Iterative Method for Solving Monotone Variational Inequality Problem with Application.	Mr.Ibrahim Arzuka
13:45-14:00	MST-O17	FIXED POINT THEOREMS FOR ENRICHED KANNAN MAPPINGS IN CAT(0) SPACES	Mr.Adamu Yusuf Inuwa
14:00-14:15	MST-O18	A NEW ALGORITHM TO GENERATE FRACTALS VIA THREE-STEP FIXED POINT ITERATIVE SCHEME FOR COMPLEX-VALUED FUNCTION	Ms.Rimsha Babar
14:15-14:30	MST-O19	ON NEW JUNGCK-TYPE ITERATIVE SCHEME WITH STRONG CONVERGENCE TO A POINT OF COINCIDENCE	Mr.Nabaraj Adhikari

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PLENARY SPEAKERS

Plenary 1

Cross-modal understanding and generation of multimodal content

Prof. Dr. Nicu Sebe

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Video generation consists of generating a video sequence so that an object in a source image is animated according to some external information (a conditioning label, a driving video, a piece of text). In this talk I will present some of our recent achievements addressing generating videos without using any annotation or prior information about the specific object to animate. Once trained on a set of videos depicting objects of the same category (e.g. faces, human bodies), our method can be applied to any object of this class. Based on this, I will present our framework to train game-engine-like neural models, solely from monocular annotated videos. The result —a Learnable Game Engine (LGE)— maintains states of the scene, objects and agents in it, and enables rendering the environment from a controllable viewpoint. Similarly to a game engine, it models the logic of the game and the underlying rules of physics, to make it possible for a user to play the game by specifying both high- and low-level action sequences. The LGE can also unlock the director's mode, where the game is played by plotting behind the scenes, specifying high-level actions and goals for the agents in the form of language and desired states. This requires learning "game AI", encapsulated by our animation model, to navigate the scene using high-level constraints, play against an adversary, devise the strategy to win a point.

Keywords: Video Generation, Image Animation, Playable environments

Plenary 2

CONTROL AND MACHINE LEARNING

Prof. Dr. Enrique Zuazua

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In this lecture we shall present some recent results on the interplay between control and Machine Learning, and more precisely, Supervised Learning, Universal Approximation and Normalizing flows. We adopt the perspective of the simultaneous or ensemble control of systems of Residual Neural Networks (ResNets). Roughly, each item to be classified corresponds to a different initial datum for the Cauchy problem of the ResNets, leading to an ensemble of solutions to be driven to the corresponding targets, associated to the labels, by means of the same control. We present a genuinely nonlinear and constructive method, allowing to show that such an ambitious goal can be achieved, estimating the complexity of the control strategies. This property is rarely fulfilled by the classical dynamical systems in Mechanics and the very nonlinear nature of the activation function governing the ResNet dynamics plays a determinant role. It allows deforming half of the phase space while the other half remains invariant, a property that classical models in mechanics do not fulfill. The turnpike property is also analyzed in this context, showing that a suitable choice of the cost functional used to train the ResNet leads to more stable and robust dynamics. This lecture is inspired in joint work, among others, with Borjan Geshkovski (MIT), Domènec Ruiz-Balet (IC, London), Martin Hernandez (FAU) and Antonio Alvarez (UAM).

Keywords: Dynamics, Control, Machine Learning and Numerics

MST-I1

Using Maple for computing exponential integrals over polytopes

Prof. Dr. Thorsten Dickhaus

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Exponential integrals over polytopes play an important role in probability theory and statistics, because they can be interpreted as joint probabilities of linear combinations of exponentially distributed random variables. Some analytical results concerning the computation of such integrals are available in the literature. However, their application requires solving a system of inequalities that characterizes the integration region. This can become quite challenging, already in small or moderately large dimensions. We demonstrate how a computer algebra system such as Maple can be used to automize the different necessary computational steps. Furthermore, we present some concrete examples, together with applications in statistics.

Keywords: Computer algebra, exponential distribution, statistical applications, systems of inequalities.

MST-I2

SOME PROJECTION METHODS WITH LINE-SEARCH RULES FOR NONLINEAR PROBLEMS IN HILBERT SPACES

Prof. Dr. Yeol Je Cho

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In 2002, Byrne proposed the projection method, which is called the CQ-algorithm, for solving the split feasibility problem in Hilbert spaces. In fact, in 1994, Censor and Elfving introduced the split feasibility problem in Euclidean spaces, which has been applied to image reconstruction, signal recovery, intensity-modulated radiation therapy and others by many authors. In this talk, we introduce some relaxed CQ-algorithms with line-search rules in Hilbert spaces to improve Byrne's CQ-algorithm in some ways and prove some convergence theorems by using the proposed algorithms. Finally, we give some numerical examples in signal processing to illustrate the main results in this talk.

Keywords:

Split feasibility problem, The CQ-algorithm, Projection method, The line-search rule, Signal processing

Mathematics Subject Classification: 47H10, 54H25, 65K05, 90C25, 90C30

MST-I3

Key results and recent advances in Dynamic Geometry

Assoc. Prof. Ovidiu Bagdasar

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Iterative processes play a fundamental role in many areas of mathematics research and practice. Examples include the numerical solution of equations, fixed-point theory, or machine learning, but also in social processes like feedback loops, trial & error, or the development of prototypes.

Dynamic geometry is primarily concerned with processes defined in the complex plane, in which, starting from a given configuration F_0 and a sequence of transformations $(T_n)_{n\geq 0}$, one obtains the configuration F_{n+1} by applying the transformation T_n to shape F_n, that is $F_{n+1}=T_n(F_n)$**.** Several questions now arise: 1) Can we find the exact shape after *n* iterations? 2) Does the sequence $(F_n)_{n\geq 0}$ converge to a fixed configuration? 3) Does $(F_n)_{n\geq 0}$ converge to a fixed shape? 4) If convergent, can we identify the limit of $(F_n)_{n\geq 0}$? 5) Can we recover the initial configuration based on the configuration obtained after *n* steps the information on the iterations $(T_n)_{n\geq 0}$, and?

These questions will be discussed in the context of simple but surprising triangle iterations, like the dynamic geometries generated by the incircle/circumcircle of a triangle, the orthic triangle, the bisector triangle, the incentral triangle, or by cevians defined with points on the power curve.

Then, we will discuss recent results involving Kasner quadrilaterals with a complex parameter. For a real number α and an initial quadrilateral $A_0B_0C_0D_0$, one can construct the quadrilateral $A_1B_1C_1D_1$ such that A_1, B_1, C_1 and D_1 divide the segments $[A_0B_0]$, $[B_0C_0]$, $[C_0D_0]$ and $[D_0A_0]$ respectively, in the ratio $1-\alpha : \alpha$. Continuing this process we obtain a sequence $A_nB_nC_nD_n$, $n\geq 0$, whose terms are called Kasner quadrilaterals (after E. Kasner (1878-1955). Here we study the parameter values resulting in convergent, divergent, periodic, or dense Kasner iterations.

Finally, we give connections to fixed-point theory, non-expansive mappins and explainable AI.

Keywords:

Dynamic geometry, iterative processes, power curve, Kasner polygons, asymptotic behaviour.

MST-I4

Strong Convergence of Alternated Inertial CQ Relaxed Method with Application in Signal Recovery

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This article proposes a strong convergence CQ relaxed iterative method with alternated inertial extrapolation step in a real Hilbert space. The propose method converges strongly under some suitable and easy to verify assumptions. Moreover, the proposed method does not require the prior knowledge of the operator norm or estimate of the matrix norm. Instead, the stepsize is self adaptive with a simple selection procedure that does not involve any linesearch procedure. Numerical ex- periments to illustrate the computational performance together with implementation of the proposed method in signal recovery application is presented. Additionally, comparison of the method with some existing iterative methods in the literature is performed.

Keywords:

Split feasibility problem, Strong convergence, Half-space, Inertial technique, Inverse problem, Compressed sensing.

MST-I5

AN OUTER QUADRATIC APPROXIMATION METHOD FOR SOLVING SPLIT FEASIBILITY PROBLEMS

Dr. Guash Haile Taddele

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In this paper we consider the multiple-sets split feasibility problem in real Hilbert space and propose a self-adaptive method that uses projections onto quadratic (balls) approximations of the problem's associated sets. Our algorithm has several major advantages over existing methods in the literature, the first is its simple implementation as it uses closed-formula projection onto balls, second strong convergence is obtained under mild conditions.

Keywords: Split Feasibility Problem; Projection Method; Balls Approximation; Strong Convergence

PHQ-I1

IMAGINARY TIME AND TEMPERATURE

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Time is used in physics as the most fundamental quantity, to describe motion and dynamics. At classical level, it forms spacetime whose dynamics is gravity. At quantum level, time serves as dynamical variable of unitary evolution. It will be discussed how imaginary time leads to both known physics in different area and new physics including temperature of black hole via the path integral formalism.

Keywords: Imaginary time, temperature, path integral.

PHQ-I2

QUANTUM SAMPLING ADVANTAGE: HOW TO PROVE IT AND DOES IT MATTER?

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For near-term quantum devices far from the error-correctable regime, natural candidates for demonstrating quantum computational advantage can be found in noisy sampling tasks that are believed to be classically intractable based on a certain complexity-theoretic assumption.

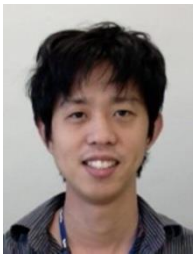
In this talk, I will compare and contrast two quantum sampling advantage schemes introduced in my works [Quantum Sci. Technol. **8** 025019] [PRX Quantum 3, 020328] situated at opposite ends of a spectrum. The first scheme pertains to a wide range of driven quantum many-body systems, but the classical intractability relies on a physical conjecture relating statistical properties of such systems to a class of random matrices, which we corroborate by numerical simulations of driven disordered Ising chain and driven Bose-Hubbard model. The second scheme, in contrast, is carefully designed to provide robust hardness guarantees comparable to those of random circuit sampling. The scheme, dubbed Fermion Sampling, utilizes a restricted fermionic gate set and specially prepared input states, is suitable for experimental realization due to the facts that number-preserving fermionic gates can be implemented with high fidelity in a superconducting qubit architecture, and the low-dimensional structure of fermionic gates allows an efficient, indirect certification of the quantum advantage scheme.

Finally, I will discuss whether these provable quantum advantages matter in near-term applications of quantum computing.

Keywords: Quantum computing, quantum advantage, quantum many-body systems

PHQ-I3

COMBINING MLFF WITH DFT: EXAMPLES OF MXENES AND TMDS



Assoc. Prof. Dr. Adisak Boonchun

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In the field of materials computational physics, both Transition-metal dichalcogenides (TMDs) monolayers MX_2 (M=Mo, W; X=S, Se, Te) and MXenes ($M_{n+1}X_n$) are of significant interest due to their potential applications in various electronic devices, supercapacitors, Li-ion batteries, and sensors. However, predicting the structural, electronic, and thermal properties of these materials using traditional density functional theory (DFT) calculations can be computationally expensive and time-consuming. To overcome this challenge, machine learning force fields (MLFFs) have recently emerged as a promising alternative that reduces computational costs while maintaining accuracy. Using on-the-fly MLFFs as implemented in Vienna Ab initio Simulation Package (VASP) code, we revealed the predictions of thermal conductivities at various temperatures, total energies at different volumes, and phonon dispersions of TMDs, demonstrating high consistency with DFT calculations. In the case of MXenes (Ti_2C and Ti_3C_2), we used MLFFs to predict the elastic and thermal properties of MXenes with different surface termination groups (O, F, and OH), offering valuable insights into the behavior of MXenes with different surface termination groups. Overall, these findings shed light on the potential of MLFFs as an effective tool for predicting materials properties, highlighting the significant role that machine learning can play in condensed matter physics and materials science.

Keywords: TMDs, Mxenes, thermal conductivity, Machine Learning Force Field

PHQ-I4

ATOMIC-SCALE DESIGN OF METAL-DIBORIDE THIN FILM-BASED HARD COATING TECHNOLOGY

Assoc. Prof. Dr. Annop Ektarawong

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Cutting tools are vitally important for machining industries, as they enable dramatic technological advancement of humankind. Presently, cutting tools are typically made out of cemented carbides and coated with an even harder material in the form of thin films, based particularly on metal nitrides and/or carbides. Besides metal nitrides and carbides, metal borides exhibiting high thermal and chemical stabilities and outstanding mechanical properties have lately been increasingly received attention from materials scientists and engineering, and they have been considered from the experimental and theoretical aspects to be promising alternatives for hard and protective coating materials for cutting tools. In this presentation, we highlight how the stabilities and the properties of metal borides can feasibly be improved through the alloying process, focusing particularly on solid solutions of $Sc_{1-x}V_xB_2$. Our investigations based on the first-principles calculations combined with the cluster-expansion method reveal that the enhancement of the stability, stiffness, shear strength, and hardness of $Sc_{1-x}V_xB_2$ solid solutions with respect to ScB_2 and VB_2 can be interpreted in terms of the electronic band filling of the bonding states of the materials.

Keywords: Transition-metal diborides; Thermodynamic stability; Mechanical Properties; ScB_2-VB_2; First-principles calculations

CHE-I1

TRANSITION METAL CO INTERACTION REVISITED WITH A TWIST OF SPIN

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The interaction between transition metal atom and CO has been a textbook example that has been rationalized by the Dewar-Chart-Duncanson model involving σ and π back donation interaction. Many previous calculations utilize density functional theory (DFT) to understand this bonding interaction. Fournier found that in the binding between 3d transition metal (TM) atoms and CO, the electronic spin state of the infinitely separated TM atom and CO have a different spin state from the TM-CO adduct. Therefore, this reaction is the most basic type of *"spin crossover"* reaction. For treating such spin crossover reactions, one usually uses the minimum energy pathway (MEP) connecting the lowest energy spin state at each relative geometry and defines an effective potential energy curve that has varying spin states along the way. The key assumption is that the electronic spin-orbit (SO) interaction is strong enough that efficient change occurs between the spin states. One thing that is forgotten here is that if the SO interaction is strong, it can greatly perturb the potential energy curve.

We focus on the Ni(triplet $3d^9 4s^1$) + CO(singlet) → NiCO (singlet Σ^+) reaction, where a triplet spin state reactant ends up as a singlet state product. First, we calculated the linear association process utilizing multireference configuration interaction (MRCI+Q) calculation based on the orbitals from 11 state average 16 electrons, 12 orbital complete active space self-consistent field method. At each Ni-C bond length, we evaluated the SO interaction and compared it with the MEP model. We found that the correct association reaction occurs through the spin crossover of Ni+CO($^3\Pi$) → NiCO($^1\Sigma^+$). Although the MEP model can give fairly good values for the heat of the reaction, the potential energy curve along the association can vary by, at most 0.2 eV. Such differences along the association potential energy curve can cause one order of magnitude change in the association reaction rate at room temperature.

Keywords: spin crossover reaction, multireference calculation, transition metal

CHE-I2

MOLECULAR/MATERIAL GENERATORS: DE NOVO DESIGN USING MODERN MACHINE LEARNING METHODS

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One of the primary objectives of computational chemistry is to identify molecules/materials that exhibit desired properties for experimental validation and potential real-life applications. This exercise involves investigating known molecules, computing/measuring properties of interest, understanding of structure-property relationships qualitatively or quantitatively and design new molecules based on this understanding. Alternatively, combinatorial methods and high-throughput screening that are more resource demanding are used. This is because of the practically infinite chemical space from that we need to explore. Last few years have witnessed the use of modern machine learning methods for addressing inverse problems that enabled us to formulate problems such as self-driving labs (see Figure below). Methods such as reinforcement learning (RL), variational autoencoder (VAE), generative adversarial network (GAN) and generative pre-trained transformer (GPT) have been used to solve inverse problems such as molecule generation, retrosynthesis, molecule characterization from spectra [1]. In this talk, we will discuss three ML frameworks that attempts to solve inverse problems. (a) MEMES: This methods uses gaussian process regression and expected improvement to make high-throughput exercise more efficient. We show that just by sampling about 5% of the database, we could identify almost 100% of all the top hits. (b) MolGPT: We show how a transformer-decoder model could be used to generate not only novel and valid molecules, but also those with desired physicochemical properties. (c) MoleGuLAR: Reinforcement learning (policy gradients) method was used for multi-objective molecule optimization. We will discuss the use of RL for de novo generation of molecules that exhibit desired multiple properties.

Keywords: Machine learning, artificial intelligence, molecule optimization, free energy

CHE-I3

MODELLING FLUORESCENCE AND PHOSPHORESCENCE FROM-FIRST-PRINCIPLES

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In this contribution I present computational protocols to model fluorescence and phosphorescence in molecular systems which go beyond the nowadays routine modelling of emission energies. Our protocols merge state-of-the-art quantum chemical calculations, excited state decay rate theories (i.e., Fermi-golden rule based) [1] along with semi-classical nonadiabatic excited state dynamics to enable the quantitative determination of fluorescence lifetimes and quantum yields. In particular, I present an extensive analysis of the parameters influencing the excited state decay rate calculations.[2] Further, protocols to model anti-Kasha fluorescence in molecular systems (i.e., fluorescence from higher-lying excited states)[3] and the first attempts to capturing fluorescence events in molecular systems within a semi-classical Non- Adiabatic Molecular Dynamics framework, [4] are presented. Finally, I present protocols to unveil the emissive species responsible for the complex phosphorescence properties of organometallic complexes.[5] These investigations contribute to our continuous efforts towards attaining quantitative determinations of photochemistry at the first principles level.

Keywords: Quantum chemical investigations, excited state decay rates, fluorescence, phosphorescence

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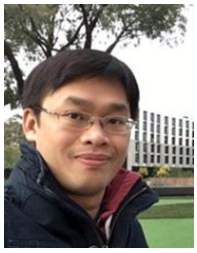
CHE-I4

ENHANCING PERFORMANCE OF V_2O_5 CATHODES IN LI-ION BATTERIES THROUGH FIRST-PRINCIPLES-BASED HETEROSTRUCTURE ENGINEERING AND CONTROLLED DOPING



Asst .Prof .Dr. Suwit Suthirakun

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Li-ion batteries (LIBs) have emerged as a well-established rechargeable energy storage technology over the past decade. However, finding a promising material for novel host electrodes remains challenging. Despite its popularity in LIBs due to low cost and high safety, V_2O_5 cathode materials still face issues of high-capacity fading and low electric conductivity. In this talk, I will explain how we can use first-principles tools to suggest strategies to improve performance of V_2O_5 cathodes. Two different strategies will be discussed: making a heterostructure and controlled doping. In particular, I will demonstrate the thermodynamic stability and improved performance of the $V_2O_5/Ti_3C_2O_2$ heterostructure compared to bulk V_2O_5. Also, Sn doping enhances electronic conductivity and facilitates the formation of a lithiated phase during Li intercalation. Overall, these findings provide insights for the design of high-performance V_2O_5-based cathode materials in LIBs, highlighting the potential of heterostructure engineering and controlled Sn doping.

Keywords: Li-ion batteries, V_2O_5, First-principles calculations, doping, heterostructure.

CHE-I5

SUPERCOMPUTER "MASAMUNE-IMR" GIVES PARADIGM SHIFTS ON SOLID OXIDE FUEL CELL SIMULATIONS

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Revealing the degradation and fracture mechanisms of solid oxide fuel cell is strongly required to make it more widespread. Therefore, the theoretical guideline for the design of high-tolerance and high-durability solid oxide fuel cells should be established. Our supercomputer "MASAMUNE-IMR" in Institute for Materials Research, Tohoku University, realizes superlarge-scale molecular dynamics simulations and gives paradigm shifts on the solid oxide fuel cell simulations. Superlarge-scale molecular dynamics simulations can clarify the effects of atomistic dynamics and chemical reactions at atomic-scale on the degradation and fracture phenomena at macro-scale. In addition, the effects of atmosphere, grain boundary, grain size, and Ni/YSZ (yttria-stabilized zirconia) composition on the degradation and fracture mechanisms can be revealed.

We performed three-million atoms simulations of Ni/YSZ electrode and successfully revealed that the smaller the size of YSZ particles, the more Ni sintering can be suppressed. Furthermore, the oxidation reaction dynamics of Ni catalysts by water molecules were clarified and their effects on the degradation and fracture processes of solid oxide fuel cell were also elucidated. In this symposium, a variety of applications of our supercomputer "MASAMUNE-IMR" to superlarge-scale molecular dynamics simulations on solid oxide fuel cell will be introduced.

Keywords: Solid oxide fuel cell, Superlarge-scale molecular dynamics simulations, Degradation and fracture mechanisms, Supercomputer "MASAMUNE-IMR"

CHE-I6

MICROSCOPIC UNDERSTANDING OF INTERFACE AT LIQUID/SOLID-OXIDE AND MOLECULAR ADSORPTION ON THE SURFACE BY NEURAL NETWORK POTENTIALS

Prof. Akira Nakayama

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The rise of the neural network potentials (NNP) for interatomic interactions has enabled the atomistic simulations of complex systems with unprecedented system sizes and long simulation times. The NNP provides a reliable description of interatomic interactions for various types of bonding with high fidelity, and by efficiently acquiring and adaptively updating training data, usually obtained by the first-principles calculations such as DFT, the NNP-based simulations are becoming a versatile tool for investigating the microscopic structure and dynamical behavior of various systems.

We will present our recent works using the NNP on the following topics:
(i) Long-range proton and hydroxide ion transfer dynamics at water/CeO_2 interface in nanosecond regime.
(ii) Grand canonical Monte Carlo simulations for the adsorption of hydrogen atoms on the metal surface and single-atom alloy.
(iii) Kinetic Monte Carlos simulations for the surface catalytic reactions with explicit treatment of the lateral interactions between adsorbates.

Keywords: neural network potential, DFT, heterogeneous catalysis, metal-oxide

CHE-I7

LITHIUM-ION SOLVATION AND TRANSPORT PROPERTIES IN BULK ORGANIC ELECTROLYTES FROM CLASSICAL MOLECULAR DYNAMICS

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Molecular dynamics (MD) simulations were employed to investigate the impact of co-solvent content and type on the solvation structure and transport properties of lithium ions (Li^+) in an electrolyte. The electrolyte consisted of lithium hexafluorophosphate ($LiPF_6$) at a concentration of 1.0 M in a carbonate-based solvent composed of ethylene carbonate (EC) and dimethyl carbonate (DMC) in a 1:1 ratio. Various co-solvents, namely tetramethylene sulfone (TMS), dimethyl sulfoxide (DMSO), fluoroethylene carbonate (FEC), and succinonitrile (SN), were incorporated into the electrolytes at different weight percentages (wt.%): 0, 10, 25, 50, 75, and 100 wt.%. The behavior of Li^+ ions was significantly influenced by the content and type of co-solvent. The highest transference number of Li^+ was observed when each co-solvent was added at a 25 wt.% concentration. Specifically, the system comprising 1.0 M $LiPF_6$ in EC:DMC = 1:1, with an additional 25 wt.% DMSO, exhibited the most elevated ionic conductivity (14.13 mS/cm) and transference number of Li^+ (0.47). Notably, in this system, the PF_6^- anion did not participate in the first solvation shell of Li^+ due to a high donor number of DMSO relative to TMS, FEC, and SN, which consequently resulted in a weakened electrostatic interaction. These simulation outcomes contribute to a fundamental understanding of the underlying principles that govern the properties of bulk electrolytes, thereby providing valuable insights for the design of electrolytes with enhanced performance and safety in lithium-ion batteries.

Keywords:
Lithium-ion battery, electrolyte, solvation, diffusion, ionic conductivity, molecular dynamics.

CHE-I8

THEORETICAL STUDIES ON THE STRUCTURES AND FUNCTIONS OF METALLOPROTEINS: TOWARDS UNDERSTANDING OF INHIBITION MECHANISMS OF CCO AND HPPD

Prof. Yasuteru Shigeta

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Proteins themselves are polymers of amino acids, which are purely organic molecules. However, they are not always functionally adequate on their own, and it is essential to enhance their functions by cofactors, especially metal ions and complexes. This is the reason why proteins have acquired more diverse functions and regulation mechanisms. Metalloenzymes catalyze various chemical reactions such as synthesis, degradation, and redox reactions under mild conditions, and the elaborate combinations of these reactions maintain the activities of life. In other words, the essence of life phenomena is a series of chemical reactions driven by them. To elucidate their reaction mechanisms at the atomic level, it is necessary to theoretically clarify the three-dimensional structure of proteins, especially the roles of amino acid residues, water molecules, and cofactors that constitute the active center. Then, the unique functions of proteins can be elucidated by comparing them with the findings by conventional biochemical and molecular biological methods. Our research group has been analyzing the functions of various metalloproteins with mutual collaborations with experimental groups. In this presentation, I will focus on the following two themes:

(1) Inhibitory mechanism of Cytochrome c Oxidase and transferability of the same idea for [1].
Cytochrome c oxidase (CcO) is the only enzyme that uses oxygen to form a proton gradient in mitochondrial oxidative phosphorylation to produce ATP. Mammalian CcO is composed of 13 different subunits, including four redox-active metal centers, two copper ions, and two heme a groups. Starting from the X-ray complex structure of CcO with a novel allosteric inhibitor discovered by Shintani et al., we performed molecular dynamics (MD) simulationsto identify its inhibition mechanism. It is shown that the inhibitor modulates the conformation of amino acids inside the protein by interacting with Helix 2, resulting in an allosteric inhibition of oxygen supply from inside the membrane to the active site. This mechanism of action applies not only to mitochondrial CcO but also to bacterial allosteric proteins. For example, it is speculated that the same mechanism may apply to specific inhibitors against ceftriaxone-resistant Neisseria gonorrhoeae. This study opens new avenues for regulating protein function and proposes an option for overcoming drug resistance.

(2) Species specific regulation of inhibition mechanism by HPPD inhibitor herbicide [2].
It is known that mesotrione as one of the HPPD inhibitor herbicides binds strongly to the broadleaf Arabidopsis HPPD, while they do not bind as strongly to the grass HPPD. The factors responsible for these differences in binding activity have not been clarified. In this study, we investigated the structural changes between Arabidopsis and Embac HPPDs based on MD in order to clarify the factors responsible for such differences in activity. Analysis of the calculation results confirmed that in the apo form without mesotrione, the inhibitor binding site of Arabidopsis HPPD is in an open state, whereas that of Embac HPPD is in a closed state covered by a-Helix at the C-terminus. This

suggests that mesotrione can easily bind to Arabidopsis HPPD, while it is difficult to bind to Embac HPPD. In the mesotrione-bound complex, the inhibitor-binding site of Arabidopsis HPPD was closed with a lid by a-Helix, whereas the inhibitor-binding site of Embac HPPD was open. Therefore, it was suggested that dissociation of mesotrione from Arabidopsis HPPD is unlikely to occur, while dissociation from Embac HPPD is likely to occur. These analyses suggest that the movement of a-Helix differs among plant species, resulting in plant-species differences in the HPPD-binding activity of HPPD-inhibitory herbicides to HPPD [2].

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Keywords
Inhibitory mechanisms by small ligand, Molecular dynamics simulations, Quantum Chemical Calculations.

CHE-I9

DISCOVERY OF Mo-B EMBEDDED C_2N AS A HIGHLY EFFICIENT ELECTROCATALYST FOR UREA PRODUCTION FROM N_2 AND CO_2 THROUGH HIGH THROUGHPUT SCREENING

Dr. Nuttapon Yodsin

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Urea (NH_2CONH_2) production by electrosynthesis at mild conditions has been considered a sustainable strategy to replace the current harsh industrial processes. However, the practical design of highly active and selective electrocatalysts for urea synthesis remains challenging. This is due to the lack of knowledge on effectively activating inert N_2 and CO_2 molecules and facilitating the formation of C-N bonds. We use density functional theory (DFT) to demonstrate that a new family of electrocatalysts with a metal−B center can boost urea production. First, we anchored a single metal atom (M = Fe, Co, Ni, Cu) on a carbon nitride nanosheet with boron (B) doping (M-B@C_2N). This surface acts as a hybrid dual−atom M–B active site for urea production from CO_2 and N_2 molecules. We evaluated all possible pathways; (i) CO_2 pathway, (ii) OCOH pathway, (iii) CO pathway, and (iv) NCON pathway on these surfaces. This systematic calculation identified the first reduction of $*N_2$ as the key step for urea synthesis. Then, we subsequentially evaluated the remaining 3d− and 4d−M doped on M-B@C_2N for this key reaction step. In addition, using the ICOHP of the $*N_2$ bond as a replacement for $\Delta G_{*N2\rightarrow *NNH}$ in the screening process has the potential to decrease computational costs, and ICOHP proves to be a promising descriptor. Through this high−throughput screening, we found that the Nb-, and Mo-B@C_2N show excellent performance with a low limiting potential of -0.56 and -0.53 V through the CO and OCOH pathways, respectively. The electronic properties along the pathway suggested that more electron transfer to the $*N_2$ moiety results in a more favorable first protonation, which is the key step for urea production.

Keywords: Density functional theory, CO_2 electroreduction, N_2 electroreduction, Urea electrochemical synthesis, C−N bond coupling

BIO-I1

DEVELOPMENT OF MOLECULAR THEORY OF SOLVATION FOR BIOMOLECULAR SYSTEMS

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Solutions play an important role as a place to produce materials and exhibit their functions. Our group has focused on the role of solutions in the formation and function of materials and has developed a multiscale method based on the statistical mechanics theory of liquids for material design.[1]

The multiscale hybrid method is effective for handling complex systems. In order to deal with electronic state changes and solvent effects in large molecular systems, the QM/MM/3D-RISM method has been proposed by us. Using this method, we have elucidated the mechanism of pKa shift caused by ligand encapsulation by macrocyclic molecules.[2]

Another important process is the change in molecular structure in solution. It is known that macromolecules, such as a polymer or protein, aggregate or phase separate under the influence of solution molecules. Recently, we have developed an efficient method for sampling molecular structures in solution. This method is designed in the framework of the hybrid Monte Carlo method: conformations are extracted at constant time intervals of MD trajectories and solvation free energies of the conformations are determined by 3D-RISM theory, and thus a metropolis criterion for conformational transitions is used. This method enables structure sampling that satisfies the 3D-RISM ensemble.[3]

These methods have been implemented in the RISMiCal package we are developing and are being prepared for releasing to the public.[4]

Keywords: 3D-RISM; QM/MM/3D-RISM; Hybrid MC

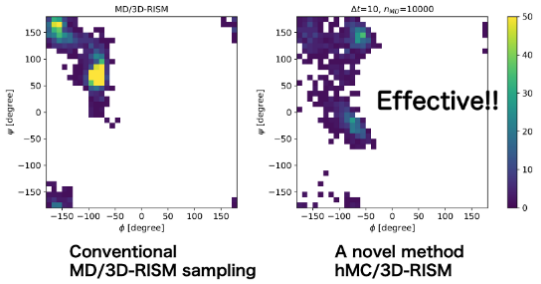

Fig. 1. Ramachandran plot of alanine dipeptide

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BIO-I2

Aggregation and disaggregation of amyloid-β peptides observed by all-atom molecular dynamics simulations

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Protein aggregates such as oligomers and amyloid fibrils cause more than 40 diseases. For example, Alzheimer's disease is caused by aggregated amyloid-β (Aβ) peptides. Aβ peptide usually consists of 40 or 42 amino acid residues. Aβ peptide with 40 residues is referred to as Aβ40, and that with 42 residues is referred to as A42. We have performed molecular dynamics (MD) simulations to understand the aggregation and disaggregation mechanisms of Aβ peptides. To analyze the aggregation process, we performed Hamiltonian replica-permutation MD simulations for Aβ40 and Aβ42 [1]. We found that the key residue for the Aβ42 dimerization is Arg5 in the oligomerization process. This residue stabilizes the β-hairpin structure and promotes the intermolecular β-sheet. We also revealed why Aβ42 aggregates faster than Aβ40. We have also performed nonequilibrium MD simulations for the protein-aggregate disruption by ultrasonic wave [2] and infrared laser irradiation [3]. We applied sinusoidal pressure to an Aβ amyloid fibril to mimic the ultrasonic wave and visualized the disaggregation process [2]. When the pressure was negative, a bubble was formed. The bubble collapsed when the pressure became positive, and water molecules crashed against the hydrophilic residues to disrupt the amyloid. We also performed nonequilibrium MD simulations in which an Aβ amyloid fibril was destroyed via infrared free-electron laser irradiation [3]. Intermolecular hydrogen bonds formed between C=O and N–H in the fibril are broken at each pulse of laser irradiation. These bonds usually spontaneously reform after the laser pulse. However, when a water molecule enters the gap between C=O and N–H, it inhibits the reformation of the hydrogen bonds. The amyloid fibril is then disrupted. In this way, we revealed different roles of water molecules in disrupting protein aggregates by the supersonic wave [2] and infrared laser irradiation [3].

Keywords
Amyloid, oligomer, molecular dynamics

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BIO-I3

COMPUTATIONAL PROTEIN DESIGN: DRIVING INNOVATION THROUGH DYNAMICS AND ENERGY OPTIMIZATION

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Computational protein design is a rapidly advancing field that holds great promise for driving innovation in the development of novel proteins with desired functions. One key aspect in this pursuit is the integration of dynamics and energy optimization methods to enhance the efficiency and effectiveness of protein design. By considering the dynamic behavior of proteins and optimizing their energy landscapes, researchers can overcome limitations in traditional static design approaches and unlock new opportunities for innovation.

In this talk, we explore the intersection of computational protein design, dynamics, and energy optimization, highlighting their collective impact on driving innovation in protein engineering. We delve into the computational techniques employed to model protein dynamics, ranging from molecular dynamics simulations to advanced sampling algorithms. Additionally, we discuss the integration of energy optimization methods, including force field parameterization, scoring functions, and optimization algorithms, to guide the design process towards energetically favourable conformations and functional outcomes.

Furthermore, we showcase how harnessing protein dynamics and energy optimization in computational design enables the creation of proteins with improved stability, enhanced functionality, and optimized binding properties. We illustrate various applications across different fields, including enzyme design, protein-protein interactions, and therapeutic protein engineering. The talk also addresses the challenges and opportunities in this evolving field, such as the accurate representation of protein dynamics, efficient exploration of conformational space, and incorporation of complex energy landscapes. We highlight emerging computational techniques and strategies that hold potential for driving further innovation in various applications, from biotechnology to drug discovery.

Keywords: Computational protein design, Computational dynamics, Energy optimization, Molecular dynamics simulations

BIO-I4

EXPLORING THE MOLECULAR MECHANISMS OF GRAPHENE QUANTUM DOT-BASED DIABETES APTASENSOR TO DETECT GLYCATED HUMAN SERUM ALBUMIN IN A SOLUTION

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Human serum albumin (HSA) is the most abundant protein carrier in blood. HSA serves as a carrier for a wide range of drugs and nutrients. A level of glycated HSA (GHSA) is used as a diabetes biomarker. A graphene-based aptasensor is one of potential techniques to detect GHSA. GHSA analytes are captured by albumin-selective fluorescent light-up aptamer which binds to dispersed graphene in a solution. The level of GHSA can be quantified by the fluorescence intensity during the release of GHSA-aptamer complex from graphene surfaces. To obtain effective GHSA aptasensor, understanding the in-depth mechanism of how aptasensor recognises GHSA becomes crucial. It is also interesting to explore the possibility of using graphene quantum dots (GQDs) for GHSA aptasensor. Thus, in this work, Molecular dynamics simulations were employed to explore key activities and properties used in GHSA aptasensor which are: (i) The nature of GHSA, (ii) How GHSA recognises aptamer, (iii) The adsorption of GHSA on GQD and aptamer-GQD (GQDA) complex. It is clear that the denaturation of albumin is detected during the assembly. Key interactions and mechanisms that GHSA utilises to adhere on GQD and GQDA are revealed. The insight obtained here will serve as a base for accurate GQD-based aptasensor design and development.

Keywords: Human serum albumin, Graphene quantum dot, Diabetes, Aptasensor, Molecular Dynamics Simulations

BIO-I5

FROM NUMBERS TO INSIGHTS: HOW MATHEMATICS EMPOWERS DISEASE SURVEILLANCE AND PREDICTION

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Mathematical analysis and modeling are at the core of infectious disease epidemiology. In this presentation, we will present an intuitive introduction to the process of disease transmission and explore the crucial roles of mathematical modeling in the field of infectious disease epidemiology, with a specific focus on its relevance to the ongoing COVID-19 transmission in Thailand. In particular, we will provide an overview of how we could model the complex stochastic transmission process using mathematical language. Additionally, we will investigate how epidemic modeling allows us to analyze the complex outbreak dynamics observed in the real world, evaluate the effectiveness of disease control measures, and project disease transmission. Throughout this presentation, we will provide a wide range of examples and case studies for the applications of epidemic modeling, from informing public health decision-making to evaluating intervention strategies. Finally, we will outline the current challenges faced in the field of mathematical epidemiology, including data limitations and the need to incorporate human behavior and societal factors, and suggest future research directions.

Keywords: Mathematical analysis, COVID-19 pandemic, Disease modeling, Computer simulation.

BIO-I6

Omics data analytic and modeling to simulate a journey of carbon conversion towards plant biomass production

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In response to the global sustainable goal 2030, sciences and technological development is essentially required for enabling the transition to climate-smart agriculture, which aims for the better climate-adaptive cultivation with more environmental friendly management. The goal cannot be achieved unless having sufficient in-depth understanding into metabolism of carbon conversion towards biomass formation, and its responsive interaction to the surrounding environment. The fundamental allows development of knowledge-based decision support tools for optimal farm management between production yielded and resource used. Centre for Agricultural Systems Biology (CASB) at KMUTT employs systems biological approach to decipher cellular regulation underlying plant growth and yield production. A variety of modeling techniques are applied to relate genetic-based intracellular responses to plant-scale physiology. Simulation of carbon conversion into plant biomass is conducted to study plant metabolic potential leading to the apparent yield distinction. The insights gained enable the prediction of carbon assimilation and allocation under prevailing environmental conditions. It allows us to estimate the environmental pressure on plant growth, which is truly benefit for choice selection of the practical treatment to secure the final harvest yield. The study of cassava root development will be presented to demonstrate the contribution of omic data analytic and crop modeling in moving a step forwards to the greener and smarter farming.

Keywords: Omics data analytic, Genome-scale metabolic modeling, Carbon conversion, Metabolism, Cassava, Storage root yield.

BIO-I7

PARALLEL CASCDE SELECTION MOLECULAR DYNAMICS FOR SAMPLING RARE EVENTS OF PROTEINS

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The biological functions of proteins are strongly related to their conformational transitions. To elucidate the essential dynamics, molecular dynamics (MD) simulation has become a powerful tool. However, it is difficult to sample the relevant conformational transitions of proteins with the conventional MD because the accessible time scales of the conventional MD are far from those of the biological functions. Furthermore, the essential transitions are induced as stochastic processes induced in the long-time scales over microseconds, meaning that the conformational transitions of proteins are regarded as biologically relevant rare events. To sample the rare events, we have proposed several rare event sampling methods. [1-2] Our strategy to sample the rare events is based on cycles of the following conformational resampling consisting of two steps. (1) Selections of essential initial structures. (2) Restarting of short-time MD simulations from the initial structures with high potential to make conformational transitions. The cycles of conformational resampling increase the transition probabilities, promoting the rare events. In this presentation, we would like to focus on our representative rare event sampling method called parallel cascade selection MD (PaCS-MD). [3] Furthermore, we would like to introduce several applications using PaCS-MD, i.e., the rare event sampling of large-amplitude domain motions of proteins and induced-fit processes upon the ligand binding.

Keywords: Protein, Rare Event, Conformational Sampling, Transition, PaCS-MD

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BIO-I8

AGGREGATION OF FULLERENES IN BIOLOGICAL MEMBRENE: MOLECULAR DYNAMICS SIMULATIONS

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Carbon nanoparticles (CNPs) are widely interesting for a great number of applications however their influence on health and environment become seriously concerns. Here, we studied on the behavior of fullerenes in plasma membrane with varying fullerene concentrations using coarse-grained molecular dynamics (CG-MD) simulations. The results showed that fullerenes spontaneously penetrate into the plasma membrane. Interestingly, fullerenes prefer to locate in the inner leaflet of the plasma membrane especially at the region of the highly unsaturated lipids. The aggregation of fullerene was observed even at low concentrations. In addition, the fullerene clusters grow, and budding may occur at the inner leaflet of the plasma membrane when fullerene concentrations increase. Our findings suggest the mechanisms of how they directly enter the cell and how fullerenes perturb cell membranes. These insights can help to determine fullerene toxicity in living cells.

Keywords
fullerene, carbon nanoparticles, biological membrane, molecular dynamics simulation.

BIO-I9

PREDICTION OF CANCER DRUG SYNERGY USING MECHANISTIC MODELING AND DEEP LEARNING

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Recent advancements in cancer treatment have focused on using drug combinations (multiple drugs employed together) rather than relying on single-drug therapies. By targeting different signaling pathways, these drug combinations have proven to be more effective in improving therapeutic outcomes. Additionally, the use of drugs with diverse mechanisms of action allows for lower individual drug doses compared to when used as single agents. However, as the number of potential small-molecule cancer inhibitors continues to grow, there is a need for in-silico strategies to predict the pharmacological synergy resulting from these combinations. In this discussion, I will explore two approaches—mechanistic modeling and deep learning—in predicting the synergy between small-molecule drugs. The mechanistic model is based on a dynamic Boolean network of protein interactions that combines cancer-specific mutations to explain the underlying mechanisms behind drug synergy. The deep-learning model utilizes the target protein profiles of the drugs as inputs to make predictions. Both models exhibit good predictive performance while providing interpretability, allowing researchers to gain insights into how protein signaling networks contribute to the observed synergistic effects when combining drugs for cancer treatment.

Keywords: Boolean network, Deep learning, Drug combinations, Model interpretability, Small-molecule inhibitors

BIO-I10

ANILINONAPHTHOQUINONES AS POTENT EGFR INHIBITORS: A COMBINED EXPERIMENTAL AND THEORETICAL STUDY

Dr. Panupong Mahalapbutr

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Epidermal growth factor receptor (EGFR) has been one of the attractive targets for targeted drug development. In the present study, a set of anilino-1,4-naphthoquinones was synthesized and investigated for their anticancer and EGFR inhibitory effects. Among 16 derivatives, compounds **3**, **8**, and **10** exhibited the most potent anticancer activity against six cancer cell lines (i.e., A549, HuCCA-1, MDA-MB-231, HepG2, MOLT-3, and T47D), the highest selectivity index, and good drug-likeness properties. From EGFR kinase assay, these three promising analogs showed strong inhibition against EGFR with the IC_{50} values in nanomolar scale, especially compound **3** containing 4-CH_3 substituent on the phenyl ring that displayed 4-fold higher potency than the erlotinib. Molecular docking, molecular dynamics simulation, and MM/GBSA-based free energy calculation revealed that van der Waals force played a major role in the protein-ligand complexation. Additionally, the 4-CH_3 moiety of the substituted benzene ring was noted to be a key chemical feature contributing to the highly potent EGFR inhibitory activity via its interactions with K745, L788, M766, T790, and A743 residues.

Keywords: Cancer, Targeted therapy, Synthesis, Computational simulation.

HPC-I1

THE DEVELOPMENT OF GOVERNMENT DIGITAL INFRASTRUCTURE WITH THE NEED OF HIGH PERFORMANCE COMPUTING SYSTEMS

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Nowadays, artificial intelligence (AI) and machine learning technologies have been applied in many areas, including science and technology, engineering, medicine, industry, trade and services as well as government. Government agencies around the world have applied AI to serve citizens in various areas such as social welfare, public health, public safety, military, transportation, education, etc. The development of AI, especially AI training, which is an important step in building an AI model, requires computing resources with high performance computing (HPC) systems. However, there will be a significant investment and maintenance costs if each individual agency invests in HPC and use only on it own. Renting HPC on cloud is also costly. Due to budget constraints, most agencies prefer to develop work in AI by using general computer systems for AI training resulting in an outcome that are inaccurate, delayed, unable to meet the needs of use. Therefore, the implementation of centralized HPC service can help the government agency to save budget on the provision of HPC resources and can also provide services quickly to meet the needs of the agency. Having centralized HPC service can also help promote the rapid development and utilization of AI and data analytic technologies among government agencies. However, building centralized HPC service is not a simple task as there are several different requirements among government agencies. There are also challenges in how to share resources efficiently and securely in a multi-tenancy environment of the centralized HPC system.

Keywords: Cloud, High Performance Computing, Artificial Intelligent, HPC, AI, Government Cloud, Digital Infrastructure.

HPC-I2

DATA-CENTRIC ACCELERATOR DESIGNS FOR HPC WORKLOADS

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The growth in modern data-intensive workloads ranging from scientific applications to AI/ML has improved the productivity of various applications. However, these applications' increasing resource demand also creates new challenges as conventional hardware and system designs fail to deliver good performance without non-trivial workarounds across diverse types of applications. This talk identifies performance bottlenecks created by popular HPC applications. Specifically, we provide an in-depth analysis of the bottlenecks in current hardware and accelerators such as GPUs. To minimize such performance bottlenecks, we introduce a combination of techniques through novel hardware designs while limiting system-level changes to allow efficient execution of these compute-intensive applications. Our proposal allows flexible hardware and enables the computing system to utilize different policies based on the applications' demand to eliminate performance pathologies and improve performance across various architectures at a low cost.

Keywords: Accelerator Design, GPUs, In-memory Processing

HPC-I3

DOES HPC MATTER? REFLECTIONS ON THE UTILITY OF SUPERCOMPUTING

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Viewed in terms of statistics, high performance computing has shown astonishing progress over the past decade. Today's top supercomputers, comprising millions of cores, generate performance benchmarks approaching or even exceeding 10^{18} (exascale) floating point operations per second. This level of computational power should make it practical to address some of the complex, multi-dimensional challenges facing humanity: modeling and mitigating climate change; predicting extreme weather events; simulating, tracking and responding to pandemics; enhancing food security and avoiding famine. Coupled with advances in machine learning technologies, HPC can produce new scientific insights by exploring huge data sets and identifying critical relationships among hundreds or thousands of variables. Together, AI and HPC promise solutions to previously intractable analytical problems in a wide range of domains.

In practice, HPC has yet to deliver on many of its promises, due to both technical and institutional factors. HPC systems are generally complex and often brittle, suffering frequent hardware faults. When they run smoothly, they consume alarming amounts of electricity. Despite their blinding speed, their computational efficiency is low. ACM Turing award winner Jack Dongarra has pointed out the today's top HPC systems achieve only a few percent of their theoretical peak performance, partly because data communication time swamps the time for computations.

Meanwhile, many of the top HPC systems belong to government organizations or corporations. Access is restricted and applications reflect the priorities of the host institution rather than more general societal needs. To reach its potential, HPC must be democratized. Educational organizations and non-profit entities must be provided with both access and technical support, and a significant fraction of the available computing power should be redirected toward applications critical for society.

To illustrate the possibilities, we will briefly introduce APEX, a supercomputer hosted at CMKL University. APEX provides an example of a flexible, accessible HPC targeting socially beneficial computational tasks.

Keywords: Exascale Computing, High Performance Computing, APEX

AIS-I1

CONCURRENT SENSING AND LEARNING WITH IN-NODE MACHINE LEARNING

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The Internet of Things, the idea that the physical world around us can be digitized, monitored and controlled, is fascinating as it complex. IoT is a mix of smart and dumb 'things', a digital ecosystem that keeps growing in size and complexity, generating a vast variety of incomplete, unstructured data. IoT is emerging as one of the biggest big-data problems at hand but is unlike any other data science projects. It is a complex spatio-temporal problem, whereby data sources are heterogeneous, unreliable, unreliably connected, and often hard to correlate. So how can we make sense of IoT data? How can we avoid turning it into an unpredictable mess? And which hurdles do we need to overcome when it comes to smart systems?

In this talk, I explore the missed potential of Cloud-based smart systems, whereby the sensed data is transferred pretty much un-processed to the Cloud. I argue that to make significant insights from IoT data, we need to initiate intelligent processes at the micro-edge (at the sensor nodes). By means of recent pilot studies, I illustrate the value of shallow learning and other lightweight learning methods, which may be employed to improve data quality and address communication and energy bottlenecks in typical smart systems. I advocate an extensive use of embedded machine learning to perform a range of data analysis tasks at the very edge of the IoT, employing intelligent processes for tasks such as data cleaning, missing-data management, compression, anomaly detection, and for self-tuning the data collection itself. All-in-all, this talk is about smart methods to enhance data quality in smart systems.

AIS-I2

EXPLORING PROBLEM SOLVING AND OPTIMIZATION: HEURISTIC, META-HEURISTIC AND HYPER-HEURISTIC SEARCH METHODS

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Heuristic, meta-heuristic, and hyper-heuristic search methods are employed in problem-solving and optimization when exact solutions are unattainable or when the problem space is complex. Heuristic search utilizes domain-specific knowledge to guide the search for solutions, employing heuristics to make informed decisions about exploration. Meta-heuristic search methods offer higher-level strategies that can be applied across diverse problem domains, often inspired by natural phenomena or human behavior. Examples of meta-heuristic algorithms include Genetic Algorithms, Simulated Annealing, Particle Swarm Optimization, and Artificial Bee Colony. Hyper-heuristic search takes automation a step further by automatically selecting or generating heuristics or meta-heuristics themselves based on predefined criteria or learning mechanisms. Hyper-heuristic algorithms create adaptable search algorithms that do not rely on domain-specific knowledge. These methods find applications in various fields, including combinatorial optimization, artificial intelligence, network routing, logistics, and more. They offer effective solutions to complex problems where exact solutions are challenging to find.

Keywords: Optimization, Heuristic, meta-heuristic, and hyper-heuristic.

AIS-I3

ACCELERATED ALGORITHMS FOR CONVEX BILEVEL OPTIMIZATION PROBLEMS AND APPLICATIONS IN DATA SCIENCE

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In this talk, we discuss some inertial and line search techniques using for accelerating the convergence behavior of the proposed algorithms for solving some convex bi-level optimization problems. We first discuss some fixed point and optimization algorithms using one and two step inertial techniques including some line search techniques for solving convex optimization problems of the form of the sum of two convex functions in which one of these functions is smooth in a real Hilbert space and then employ those algorithms as machine learning algorithms for solving some problems in data science such as regression and data classification. We also use the mentioned techniques to introduce new accelerated algorithms for solving some convex bi-level optimization problems and apply them for solving image restoration problems and some problems in data science. Convergence behavior of the proposed machine learning algorithms are also analyzed and by numerical experiments, we compare efficiency of the introduced algorithms with the existing algorithms in the literature.

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CFD-I1

Properties and Applications of Nanofluids; Theory and Mathematical Modeling

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Nanofluids, a class of engineered colloidal suspensions containing nanoparticles in a base fluid, have gained significant attention in recent years due to their unique properties and wide-ranging applications. They exhibit exceptional thermal, optical, and rheological properties compared to their base fluids. The addition of nanoparticles enhances thermal conductivity, leading to improved heat transfer characteristics. The rheological behavior of nanofluids, influenced by nanoparticle concentration, shape, and surface functionalization, affects their flow and stability, offering opportunities for tailored fluid behavior. The unique properties of nanofluids have enabled their utilization in various fields. In the realm of thermal management, nanofluids find applications in heat exchangers, electronic cooling systems, and nuclear reactors, where their enhanced thermal conductivity enhances heat dissipation. Nanofluids also find use in energy conversion and storage, including solar thermal systems, thermoelectric devices, and phase-change materials for thermal energy storage. Additionally, nanofluids have been explored in biomedical applications, such as drug delivery, hyperthermia therapy, and bioimaging, owing to their improved optical and thermophysical properties. The mathematical modeling of nanofluids plays a crucial role in understanding their behavior and optimizing their performance. Various theoretical and empirical models have been developed to describe the heat transfer and fluid flow of nanofluids. These models incorporate parameters such as nanoparticle concentration, size, shape, and thermophysical properties. Theoretical models provide insights into the fundamental mechanisms governing nanofluid behavior. Empirical correlations, derived from experimental data, offer practical tools for predicting nanofluid performance under specific conditions.

Keywords: Nanofluids, thermophysical properties, flow behavior, modeling, performance analysis

IEE-I1

Multimodal User Models for Life Enhancement

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What we learned from 7 years of competitive evaluations It is no surprise that we are all gathering increasingly large digital media archives. These can range from digital photos, biometric data, and data gathered by organisations on our behalf. The question addressed in this talk is what can happen when we bring all these data sources together into one unified multimodal archive. Over the past decade my team have been developing rich multimodal user models that unify all these data sources into a personal lifelog or memex. In this talk, I will introduce the concept of a lifelog, highlight the value that the lifelog models can bring to an individual's memory, health, education, and entertainment, and finally showcase the progress that we have made in organising and searching through these lifelog models. I will specifically focus on what we have learned from seven instances of the ACM Lifelog Search Challenge at the annual ACM ICMR conference, such as the importance of multimodal fusion and relevance feedback for lifelog search.

IEE-I2

Causality inspired retrieval of human-object interactions from video

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In this talk, the speaker will present a novel approach to retrieve human-object interactions from video data by utilizing the concept of causality. By applying causal inference methods, the aim is to detect the causal relationships between human actions and the objects present in their environment. This information is then used to develop a retrieval system that is both robust and accurate. The motivation behind this approach stems from the fact that human-object interactions are inherently causal, and understanding the causal mechanisms at play can significantly enhance retrieval performance. The talk will showcase experimental results that validate the effectiveness of the proposed approach and discuss potential applications in diverse fields such as robotics, surveillance, and human-computer interaction.

IEE-I3

CHOSEN Digital: EV and Energy Modernization Platform

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CHOSEN Digital, led by founder and CEO Worapoj Ruenrerngwong, is an innovative company that specializes in EV and Energy Modernization. CHOSEN Digital is the 1st EV and Energy Modernization Platform in Thailand and ASEAN. The company's mission is to make energy management and sales accessible to everyone. Their groundbreaking work has earned them 1st rank in Thailand Innovation Agency Strategic Fund, 1st Rank Delta Angel Fund Ministry of Industrial and 1st Rank of Startup Connect, the final round of Techstars Sustainability Paris, TOP3 of Jetro, and TOP150 from 4000+ XPITCH (the largest contest in Asia). Currently, CHOSEN Digital is developing pilot projects with the government, with plans to sign a national platform in the coming year. Their ultimate goal is to provide smart, clean energy for a better world.

Keywords: EV, Energy Modernization Platform, Clean energy

IEE-I4

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IEE-I5

Predictive Model for Assessing Lithium-Ion Battery Health in Electric Vehicles

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This research focuses on studying the estimation of state of health (SoH) for lithium-ion batteries utilizing an Artificial Neural Network (ANN). The primary objective is to examine the correlation between the DC internal resistance and the battery's SoH. A notable advantage of DC internal resistance measurement is its non-invasive nature, as it does not necessitate battery removal from the system. By analyzing degradation patterns observed during multiple cycles, the relationship between DC internal resistance and battery health is studied and subsequently employed to train the ANN. The developed ANN model is then tested on various battery packs, demonstrating acceptable error. The battery and analyzes parameters obtained from EV charging, including voltage, current, and charging time are also used to validate the propose predictive model. The analysis of experimental results reveals that as the service life of EVs increases, the charge to voltage ratio decreases. This ratio can serve as an indicator of battery health. As a result, this ANN model can serve as a valuable tool in early detection of potential battery failures caused by degradation, enabling timely interventions and maintenance actions.

ORAL PRESENTATION ABSTRACTS

MST-O1

A NOVEL SUPPORT VECTOR MACHINE WITH GENERALIZED PINBALL LOSS FOR UNCERTAIN DATA CLASSIFICATION

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In real-world problems, data suffer from measurement errors, data staleness, and repeated measurements, which make data uncertain. To consider the uncertainty of data, the concept of giving each data feature as a multi-dimensional Gaussian distribution has been utilized. In 2021, support vector machines with an insensitive zone pinball loss (UPinSVMs) for uncertain data classification was proposed, where is a positive number. The UPinSVMs bring noise insensitivity, stability for resampling, and increased model sparsity. However, the value of is known to be specified. In order to improve the performance, we combine the generalized pinball loss ((1, 2)-Mod-Pin-SVM) into the uncertain classification, term as UGPinSVMs, where 1, 2 are two positive numbers. The generalized pinball loss is an optimal insensitive zone pinball loss and is an extension of existing loss functions that also addresses the issues of noise insensitivity and resampling instability. We solve the primal quadratic programming problems by transforming individuals into unconstrained optimization using an efficient stochastic gradient descent algorithm. More specially, we have introduced verified theorems that are related to our approaches and investigated scatter minimization. The results from several benchmark datasets show that our model outperforms the existing classifier in terms of accuracy and statistical analysis. Furthermore, the application of our framework to the crop recommendation dataset is also examined.

Keywords: Support vector machine, Uncertain dataset, Noise insensitivity, Generalized pinball loss

MST-O2

SMOOTH SUPPORT VECTOR MACHINE WITH GENERALIZED PINBALL LOSS FOR PATTERN CLASSIFICATION

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The generalized pinball loss function was introduced to improve the noise sensitivity and random instability of the original support vector machine (SVM). However, because the generalized pinball loss function is not smooth, SVM that uses it (GP- loss-SVM) is non-differentiable. From this issue, it makes the several practical algorithms that cannot be used to find the solution. As a result, GP-loss-SVM performs less effectively in practice. In order to solve this problem and improve GP-loss-SVM, in this paper, we construct a new smooth approximation function of the generalized pinball loss function into the SVM. As a result, a smooth SVM with the generalized pinball loss function is obtained. Furthermore, we use an effective method, quasi- Newton–Armijo, to solve our model. Moreover, we prove that our new loss function can estimate the generalized pinball loss function. Finally, we conduct a thorough experimental investigation employing a variety of machine learning benchmark datasets. The experiment results on binary datasets show that the proposed method outperforms the original SVM method by up to 1.59% for linear kernel and 1.45% for nonlinear kernel; the experiment results on multi-class datasets show that the proposed method outperforms the baseline model by up to 1.43% for linear kernels. We also evaluate the statistical significance of the performance values attained for the various models using the Friedman test. The results demonstrate that the average rank of the proposed method is better compared to baseline models.

Keywords: Smooth support vector machine, Generalized pinball loss, Quasi- Newton–Armijo method, Smooth Generalized pinball loss function

MST-O3

LONG-RANGE CORRELATION BEHAVIOR OF RESTING-STATE EEG SIGNAL WITH APPLICATION IN MAJOR DEPRESSIVE DISORDER DIAGNOSIS

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Long-range temporal correlations (LRTC) in EEG oscillations have been reported to be associated with depressive symptoms. Several studies have utilized detrended fluctuation analysis (DFA) to analyze LRTC in the amplitude envelope of different EEG frequency bands (broad, delta, theta, alpha, beta) with different ranges of window sizes. However, the reason behind the choices of window sizes ranges was still unclear. In this study, we calculated the DFA scaling exponent and the Hurst exponent based on rescaled range statistic (R/S) methods of broadband EEG signal of a group of major depressive disorder (MDD) patients compared with a group of healthy controls. The optimal range of window sizes for the classification performance was determined. We further identified the frequency band that mainly contributed to the difference between the two groups. Results demonstrated the significant difference between the Hurst exponent of the original EEG signal of MDD patients (0.350 ± 0.059) and healthy controls (0.517 ± 0.085) (p-value < 0.001) with AUC-ROC of 0.934. The optimal range of window sizes was found to be 0.02 - 22 seconds. The huge difference was found to be in the delta frequency of EEG signals, with insignificant differences in other frequency bands. These results suggested that EEG signals of MDD patients possessed anticorrelated LRTC behavior, which was not found in healthy controls. This behavior may be associated with underlying brain physiology alteration related to depressive symptoms and can be an effective biomarker to diagnose MDD in the future.

Keywords: Long-range Temporal Correlations; Electroencephalography Signal; Detrended Fluctuation Analysis; Major Depressive Disorder; Hurst Exponent

MST-O4

PROVINCE SCALE RICE YIELD PREDICTION USING STATISTIC METHOD

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Over half of the world's population consumes rice, which is also an important source of income for many farmers. Therefore, crop yield prediction is useful for informing the expected yield accurately to help make decisions about planting and harvesting. While traditional yield forecasting systems typically rely on limited ground survey data and techniques such as supervised machine learning and statistical models to predict rice yield based on weather conditions, recent advances in free-to-use multi-time and multi-spectral remote sensing technology have provided a valuable tool for supporting these systems through accurate monitoring and estimation of pre-harvest crop yields. In order to leverage the benefits of this technology for rice yield prediction, climate data, observed rice yields, and remotely sensed data must be combined over an adequate time frame. Additionally, corresponding records of crop yields in the province should be taken into account for the development and implementation of provincial rice-yield predictions. Here, Multiple linear regression (MLR) and Ordinary Least Squares (OLS) are used in modelling to predict a response variable based on predictor variables. OLS is a specific MLR technique that estimates the model parameters (coefficients) by minimizing the sum of the squared errors between the predicted and actual values of the dependent variable. The weather conditions such as humidity, temperature, rainfall and Normalized Difference Vegetation Index (NDVI) are needed to use as predictors when predicting rice yield. Rice dataset was divided into 2 seasons that are in-season rice (na pi) and of-season rice (na prang). Each season has 6 types - Thai Hom Mali (in area), Thai Hom Mali (outer area), white rice, Pathum Thani 1, glutinous rice and others paddy where each type has different characteristics. The model's performance was evaluated using mean absolute percentage error (MAPE). The results show that we can predict in-season rice with high degree of correspondence with actual yield levels. On the contrary, the prediction of off-season rice using the available data poses a greater challenge, although the outcomes still exhibit a satisfactory level of performance.

Keywords: rice; yield prediction; statistical model; remote sensing; NDVI

MST-O5

AN INTEGRATED PICKUP AND DELIVERY PROBLEM AND FEEDER VEHICLE ROUTING PROBLEM

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A pickup and delivery problem (PDP) involves the movement of goods or people from one location to another, which has become increasingly important in recent years due to the growth of online shopping and home delivery services. This problem aims to route vehicles that can serve the goods to a customer in the time windows. However, the transportation problem in cities is becoming increasingly complicated due to the high population density and congestion. This problem requires effective and efficient routing algorithms to manage vehicle fleets. Many researchers have developed the feeder vehicle routing problem (FVRP) to address this issue, which allows for using different vehicles in specific regions. Therefore, we study the integration of the PDP and the FVRP to solve the pickup and delivery problem in urban. A new mathematical model is proposed, which aims to optimize the routing of vehicles for both pickup and delivery tasks while also considering the use of different vehicle sizes for different regions. The proposed model is tested using a simulated case study in a major city. The research findings are expected to significantly affect the transportation industry, particularly in urban logistics and last-mile delivery services.

Keywords: Vehicle Routing Problem; Pickup and Delivery Problem; Feeder Vehicle Routing Problem; Mixed Integer Linear Programming Model

MST-O6

IMAGE INPAINTING VIA THE MODIFIED EXEMPLAR-BASED INPAINTING WITH TWO-STAGE STRUCTURE-TENSOR AND IMAGE SPARSE REPRESENTATION

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The approach described in this research is an exemplar-based inpainting problem that combines a two-stage structure-tensor and image sparse representation to fill in any missing pixels. An important step is to select the filling order and local intensity smoothness, as well as to ensure that the structure is not destroyed. We employ a two-stage structure-tensor-based priority for the filling order. The second finding the candidate patch and determining the appropriate weight of each candidate patch under the constraint of local patch consistency, then applying a blend of a sparse linear combination of candidate patches to fill in the missing region of the image. In addition, this technique may also be used for object removal. Comparisons of performance reveal that the proposed strategy performs more effectively than the previous algorithms.

Keywords: Image Inpainting; Exemplar-Based Inpainting; Sparse Representation; Texture Synthesis; Structure-tensor.

MST-O7

A MIXED-INTEGER LINEAR PROGRAMMING MODEL FOR SOLVING A MULTI-DEPOT INVENTORY ROUTING PROBLEM WITH PERISHABLE PRODUCTS

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This paper presents a mixed-integer linear programming (MILP) model to solve the multi-depot inventory routing problem with perishable products. This problem considers delivering a single product from multiple depots to several customers to meet customers' demands in each period through transportation using a homogeneous vehicle with the same capacity. Since the products shipped are perishable, the product's shelf life must be considered. The proposed model aims to determine the delivery routes, the number of products produced, and the inventory level at the depot at different times with the minimum cost. A case study is illustrated to show the results obtained from the proposed model, and the small problems were generated and solved using the CPLEX solver that can be solved in a reasonable time.

Keywords: Perishable products; Mixed-integer linear programming model; Inventory routing problem

MST-O8

EKELAND'S VARIATIONAL PRINCIPLE ON NON-TRIANGULAR METRIC SPACES

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In this paper, we introduce Ekeland's variational principle on non-triangular metric space. We applied the proposed variational principles to obtain existence theorems for a class of equilibrium problems. Finally, we deduce the existence of equilibrium reformulation.

Keywords: Ekeland's Variational Principle; Equilibrium Problem; Non-triangular metric space.

MST-O9

A CONJUGATE GRADIENT METHOD WITH NON-MONOTONE-BASED LINE SEARCH FOR LARGE-SCALE PROBLEMS WITH APPLICATION TO NON-NEGATIVE MATRIX FACTORIZATION PROBLEMS

P. Presenter (Mahmoud M Yahaya)[1,2], Parin Chaipunya[1,2], and Poom Kumam [2]*

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Conjugate gradient CG has recently gained more traction for large-scale problems due to its unique characteristics, such as low-memory requirement and simple implementation. It is well-known that two compartments that define a CG method are: step-length α_k and the search direction d_k (which has in its formulation a β_k parameter - a crucial component of CG method) and on the other hand, still, most researchers of CG methods focus on just developing the β_k term with little concern giving to innovating on the α_k front. Thus, they mainly use the classical monotone line search (LS), such as the Wolfe line search approach to computing the step size, α_k; however, this LS approach is computationally demanding and was shown to creep in for problems with a curved narrow valley. To mitigate these shortcomings, In this article, we introduce a non-monotone LS approach that is computationally efficient--Thus, suitable for large-scale problems. Moreover, we coined a new CG parameter based on scaled Polyak Rebiere Polyak, PRP term. Hence, a new non-monotone CG method is introduced, and under some mild assumptions, the method was shown to be sufficiently decent and proved globally convergent. Finally, the scheme was tested on diverse benchmark problems taken from the CUTEst library, and we subsequently applied it to non-negative matrix factorization problems.

Keywords: Non-monotone line search; conjugate gradient; non-negative matrix factorization; conjugate gradient parameter; line search strategy.

MST-O10

MODIFIED CONJUGATE GRADIENT METHODS FOR VECTOR OPTIMIZATION

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Conjugate gradient (CG) methods are often the most efficient and effective methods due to their simplicity and low-memory requirement, especially when the dimension of the variables is large. Using Wolfe conditions, the formulated Fletcher-Reeves (FR) and Hesteness-Stiefel (HS) CG methods in the vector setting could not produce sufficient descent conditions for their global convergence. Thus, it remains an open problem. In this work, we proposed the modified FR and HS CG methods to have this important property. We establish the global convergence of the proposed methods. For comparison, we present some numerical experiments to show the implementation, efficiency, and robustness of the proposed methods.

Keywords: Conjugate gradient method; Multiobjective optimization; Pareto-optimality; Vector optimization

MST-O11

CONVERGENCE RESULTS ON A NEW CLASS OF MULTI-VALUED GENERALIZED NONEXPANSIVE MAPPINGS IN BANACH SPACES

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In this work, we introduce a new class of multi-valued generalized nonexpansive mappings. We establish some convergence results for these mappings in uniformly convex Banach spaces using the multi-valued version of a known iteration process in literature. Also, we present a numerical example to support our results.

Keywords: Fixed point; Multi-valued generalized nonexpansive mappings; Uniformly convex Banach space; Strong convergence; Iteration process

MST-O12

Inertial CQ-algorithms for k-strict pseudo-contractive mappings in Hilbert Spaces

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In this work, we introduce and study two inertial CQ-inertial algorithms for approximating some fixed points of a k-strict pseudo-contractive mapping in Hilbert spaces. An inertial hybrid algorithm is developed in order to obtain strong convergence by utilizing the inertial extrapolation method mixed with the convex combination of three iterated vectors.

Keywords: Inertial hybrid algorithm, CQ-algorithm, k-strict pseudo-contractive,

MST-O13

A HYBRID METHOD FOR GENERALIZED MIXED EQUILIBRIUM PROBLEMS, ZERO PROBLEMS AND FIXED POINTS OF ASYMPTOTICALLY DEMICONTRACTIVE MAPPINGS IN THE INTERMEDIATE SENSE

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In this paper, we introduce a hybrid projection algorithm for approximating a common element in the set of solutions to a system of generalized mixed equilibrium problems with relaxed β - α monotone mappings, common fixed points of a countable family of equally continuous and asymptotically demicontractive mappings in the intermediate sense and of null spaces of a countable family of i - inverse strongly monotone mappings in a real Hilbert space. We also established a strong convergence theorem of the algorithm. We further give numerical examples to show the performance of our algorithm and justify that our scheme is more effective and implementable. Our result is an improvement of many recent results in the literature.

Keywords: Asymptotically Demicontractive map in the intermediate sense; Relaxed Monotone Mapping; Zeros Problems; Equilibrium Problems; Fixed Point Problems.

MST-O14

ON NEW JUNGCK-TYPE ITERATIVE SCHEME WITH STRONG CONVERGENCE TO A POINT OF COINCIDENCE

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The convergence theorem for approximating a coincidence point or a common fixed point of two given mappings is a valuable result with several benefits. One of the many benefits is that it provides a systematic and reliable method for finding a common fixed point in specific scenarios. Moreover, the convergence theorem can offer computational advantages. Utilizing the iterative process described in the theorem makes it possible to approximate the common fixed point without resorting to exhaustive search or trial-and-error methods. This can significantly reduce computational complexity and improve efficiency. This research aims to introduce a novel three-step iteration approach of Jungck-type to approximate a coincidence point of two non-self-mappings $S,T:Y\to X$, where X is a normed space and Y is any set with $T(Y)\subseteq S(Y)$ and $S(Y)$ is a complete subspace of X, under some specific conditions on S and T. In this case, if $X=Y$, we obtain a convergence theorem for approximating a common fixed point of S and T. Moreover, we establish the stability result for a pair of non-self mappings satisfying the focusses contractive condition and investigate the convergence rate of our proposed iteration in Banach spaces.

Keywords: Banach Spaces; Coincidence points; Fixed points; Stability; Strong convergence

MST-O15

NEW NORMAL OPERATOR AND ITS PROPERTIES ON CAT(0) SPACES

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In this paper, we discuss about convexity, quasiconvexity, and other new property on CAT(0) spaces. Moreover, we will introduce a new normal operator in quasiconvex optimization on CAT(0) spaces by developing from the adjusted normal operator from Banach space, which was introduced by Aussel Didier in 2014. Especially, we have shown that our normal operator is monotone on CAT(0) spaces.

Keywords: Quasiconvexity, Normal Operator, CAT(0) spaces

MST-O16

Iterative Method for Solving Monotone Variational Inequality Problem with Application

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In this work, we propose two algorithms for solving variational inequality problems over the set of fixed points of nonexpansive mapping. The operator involved is monotone and Lipstchitz continuous. Moreover, each of the proposed algorithms uses two conjugate gradient-like directions. The directions facilitate the convergence of the iterates to the fixed point of the nonexpansive mapping and the solution of the variational inequality problem. We establish strong convergence of the iterates generated by the algorithms and illustrate the computational advantages of the algorithms with several numerical examples. Lastly, we demonstrate the potential application of the proposed algorithms in recovering original images from degraded ones.

Keywords: Variational Inequality; Conjugate Gradient Method; Monotone Operators; Fixed Point; Nonexpansive Mapping

MST-O17

FIXED POINT THEOREMS FOR ENRICHED KANNAN MAPPINGS IN CAT(0) SPACES

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This article presents enriched Kannan and enriched Bianchini mappings in the framework of unique geodesic spaces. For such mappings, we establish the existence and uniqueness of fixed point in the setting of CAT(0) spaces, and show that an appropriate Krasnoselskii scheme converges with certain rate to the fixed point. We proved some inclusion relations between enriched Kannan mapping and some applicable mappings such as strongly demicontractive mapping. Finally, we give an example in a nonlinear CAT(0) space and perform numerical experiments to support the theoretical results.

Keywords: CAT(0) space; enriched Bianchini mapping; enriched Kannan Mapping; fixed point; Kransnoslskij iteration; strongly demicontractive mapping.

MST-O18

A NEW ALGORITHM TO GENERATE FRACTALS VIA THREE-STEP FIXED POINT ITERATIVE SCHEME FOR COMPLEX-VALUED FUNCTION

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Fractals are an important part of modeling the natural world. The current point is to explore the escape criteria to create specific fractals. The purpose of this research is to invent a new algorithm to generate some beautiful fractals by applying a three-step fixed point iterative scheme to generate Julia set and Mandelbrot set for complex-valued function $\sin(z^n)+ az +c$, where $a, c \in C$, $n \in N$ with $n \leq 2$, and z is a complex variable with the help of escape criteria of the proposed iterative method for different situations. In addition, we examine the engrossing behavior of Julia set and Mandelbrot set for various n at certain fixed input parameter points.

Keywords: Complex-valued functions; Julia set; Mandelbrot set; Escape criterion

MST-O19

ON NEW JUNGCK-TYPE ITERATIVE SCHEME WITH STRONG CONVERGENCE TO A POINT OF COINCIDENCE

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In order to approximate a point of coincidence of two non-self mappings satisfying some contractive-like condition, a novel three-step Jungck-type iteration approach is proposed in this study. Additionally, we prove the stability result for a pair of non-self mappings under a particular contractive condition in Banach spaces.

Keywords: Coincidence points; Banach Spaces; Fixed points; Strong convergence; Stability

PHQ-O1

NUMERICAL RELATIVITY SIMULATION OF BINARY BLACK HOLE MERGER

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With the advent of an open-source SENR/NRPy+ code, one can do numerical relativity simulations on a personal computer. The SENR/NRPy+ code has capability in translating user-friendly, python script, encoding a set of mathematical equations in general relativity expressed in Einstein's tensorial forms, to highly optimized C code for unleashing computational speed of the personal computer. In this talk I will present a simulation of binary black hole (BBH) merger as an example. Based on the Arnowitt-Deser-Misner (ADM) variables for the initial data of BBH, a well-posed evolution of the Einstein equations is done through the Baumgarte-Shapiro-Shibata-Nakamura formalism. Simulation of the BBH merger is validated through convergence to zero of the Hamiltonian constraint violation. Finally, remnants of the BBH merger exhibit a ringdown gravitational wave signal.

Keywords: ADM variables, Binary black hole; BSSN formalism; Numerical relativity; SENR/NRPy+

PHQ-O2

A COMPARISON OF QUANTUM GRADIENTS

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Quantum gradient is one of the important processes in Quantum optimization that may reduce the time spent on work as well as increase the accuracy of the results from classical optimization method. It consists of several steps; data encoding, modeling, problem formulation, and updating parameters. The study revealed the process of transforming the problem into quantum circuit and compared 5 different gradient methods for updating parameters; Parameter shift rule, Finite difference, Linear combination of unitaries, Quantum natural gradient, and Quantum newton gradient with various problems; Max-cut, Clique, Binary linear programming, and Knapsack. The results showed that Linear combination of unitaries is the fastest in terms of runtime, and Finite difference is sensitive to noise.

Keywords: Quantum computing; Quantum optimization; Quantum machine learning; Circuit learning;

PHQ-O3

ACCURACY OF COARSE-GRAINED MARTINI MODEL IN PREDICTING NANOPARTICLE DIFFUSION COEFFICIENTS: A COMPARATIVE STUDY FOR OLEIC-MAGNETITE NANOPARTICLES

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The relevance of diffusion coefficient is crucial in designing nanoparticles for research, as it can be obtained through molecular dynamics (MDs) simulation. As such, simulating realistic all-atom models is computationally expensive. To address the issue, a coarse-grained MARTINI model is employed for both nanoparticle and solvent with a proper validation by comparing bond length and angle distributions between all-atom and coarse-grained MARTINI model. However, the accuracy of coarse-grained model for determining diffusion coefficient has not been assessed, especially for long chain ligands such as oleic acid. To validate the model, we use mean-squared displacement (MSD) to calculate and compare the diffusion coefficients and hydrodynamic radius in both all-atom and coarse-grained models. In the system with coarse-grained water, the hydrodynamic radius obtained from diffusion coefficient is off due to inconsistency in viscosity of the water. In contrast to all-atom water, the hydrodynamic radius between all-atom and coarse-grained models of nanoparticle are statistically the same. To justify the inconsistency, a new dynamic viscosity is determined by the periodic perturbation method via cosine-shaped periodic acceleration, and a new hydrodynamic radius is addressed.

Keywords: nanoparticle, diffusion coefficient, coarse-grained MARTINI model, mean-squared displacement (MSD), cosine-periodic perturbation method

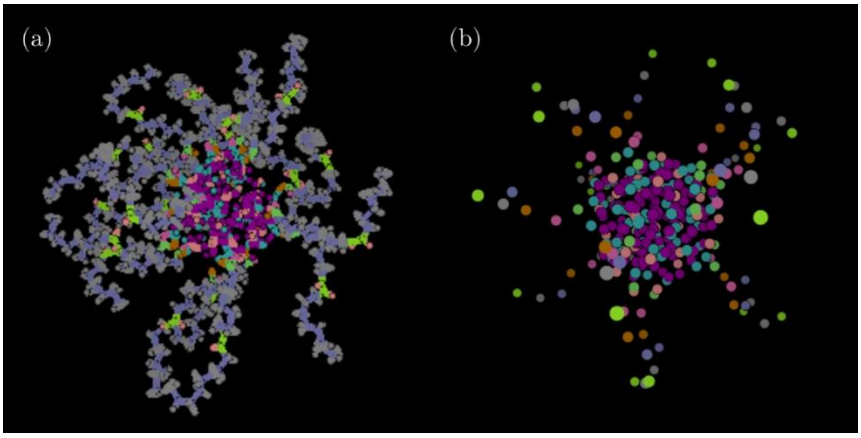

Figure 1 (a) All-atom model and (b) coarse-grained MARTINI model of oleic-magnetite nanoparticle

PHQ-O4

FREQUENCY-DOMAIN INVERSION OF TERAHERTZ INTENSITY DATA USING A HYBRID MODELING METHOD

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Imaging using electromagnetic waves in terahertz (THz) frequency range (0.1 – 10 THz) has drawn much attention during the last few decades as it offers unique properties and advantages compared with waves in other frequency regimes. Computed tomography and diffraction tomography are ones of the well-known THz imaging techniques. They are formulated mathematically based on an inverse problem where internal structures and physical properties of objects of interest are reconstructed from scattered THz waves. However, such traditional inversion methods are not suitable for materials with high-refractive index due to the use of simplified wave propagation model. Additionally, in some acquisition systems, only intensity information can be measured. This work aims to address these challenges by developing a non-linear full-waveform inversion (FWI) method for reconstructing highly-heterogeneous distribution of refractive index of the objects using only intensity data. The intensity data was simulated as if it was acquired from a THz continuous-wave (THz-CW) system emitting waves at a frequency of 0.1 THz. In this work, the scattered field in a small region surrounding the target is computed by solving the Helmholtz equation using the finite-difference method. The scattered field is then extrapolated to the positions of receivers, located in the air far from the target, using the Lippmann-Schwinger equation. This hybrid method is considerably more efficient in computing the scattered fields than solving the Helmholtz equation for the entire domain. Reconstruction results from simulated datasets show promise in estimating the shapes and refractive index values of objects. Feasibility and performance of the proposed method need to be investigated on the real datasets.

Keywords: THz imaging; inverse problem; numerical optimization; full-waveform inversion; finite-difference frequency-domain

PHQ-O5

SIMULATION OF PLASMA OPERATION WITH SMBI FUELING IN OHMIC MODE FOR THE THAILAND TOKAMAK-1 USING THE TASK/TR INTEGRATED MODELING CODE

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This study uses TASK/TR integrated modeling code to computationally investigate plasma operation scenarios on the Thailand Tokamak-1 (TT-1) in Ohmic mode, focusing on the effectiveness of Supersonic Molecular Beam Injection (SMBI) as a fueling method. The SMBI is proposed in TT-1 to deliver more efficiently and deeply fueling gas compared to traditional gas puffing methods. The simulations are carried out under various plasma conditions, including a major radius of 65 cm, a minor radius of 20 cm, a magnetic field in the range of 1.0 - 1.5 T, an electron density of $1x10^{19}$ – $5x10^{19}$ m^{-3}, and a plasma current in the range of 40-150 kA. Using TASK/TR, we calculate continuous particle sources of hydrogen gas assuming SMBI fueling and observe the resulting increase in particle distribution throughout the tokamak. Our findings suggest that SMBI could offer improved fueling capabilities for the Thailand Tokamak-1.

Keywords: Thailand Tokamak 1; Supersonic Molecular Beam Injection; Fusion Energy; TASK/TR

PHQ-O6

STUDYING THE BEHAVIOR OF CHARGE CARRIERS IN THIN-FILM PEROVSKITE DEVICES UNDER PRE-BIAS SPACE-CHARGE-LIMITED CURRENT MEASUREMENTS BY MEANS OF DRIFT–DIFFUSION SIMULATIONS

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Metal halide perovskites have a high potential for applications in optoelectronic devices. However, the practical use of metal halide perovskites is still a challenge due to the movement of mobile ions in these materials. Pre-bias space-charge-limited current (SCLC) measurement, which was recently introduced, is a technique for studying charge transport in metal halide perovskites by reducing mobile ion motion. However, a better understanding and accurate interpretation of the pre-bias SCLC results are needed. To gain insights into charge transport behaviors in pre-bias SCLC measurement results, we use drift-diffusion (DD) simulation to study the ion distribution profile and the effect of mobile ions, intrinsic charge carrier traps, and ionic traps in hole-only devices. We develop an analytical model to explain current density-voltage curves under pre-bias SCLC measurements. Using pre-bias SCLC together with our newly developed analytical expression will be useful to experimentalists as a new method for studying charge transport in perovskite materials.

Keywords: SCLC measurement; Drift–Diffusion; Hole-only device; Perovskite; Ion-migration.

CHE-O1

EXPLORING THE IMPACT OF Fe DOPING ON THE ELECTROCATALYTIC ACTIVITY OF NIOOH FOR HMF-TO-FDCA OXIDATION: A FIRST-PRINCIPLES APPROACH

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The electrochemical oxidation of hydroxymethylfurfural (HMF) involves the conversion of HMF to 2,5-furandicarboxylic acid (FDCA), which serves as a precursor to produce bio-based materials. Recent studies have developed numerous Ni-based electrocatalysts that have shown high efficiency in oxidizing HMF to FDCA. Ni-based electrocatalysts can be improved by doping NiOOH with Fe; however, the exact role of Fe is still under debate. In this talk, we will discuss how a first-principles approach can be used to explore the impact of Fe on the enhanced electrocatalytic activity of NiOOH toward HMF-to-FDCA oxidation. In particular, we will explain magnetic properties of the NiOOH model catalyst based on its calculated electronic structures and magnetic configurations. The model was then used to study HMF oxidation mechanisms where all key intermediates were considered. Lastly, the effect of Fe doping on the electronic-magnetic properties and reaction mechanisms will be discussed. The obtained knowledge from this study can be used to rational design doping strategies to enhance catalytic performance of NiOOH based electrocatalysts.

Keywords: NiOOH; NiFeOOH; Fe doping; HMF electrochemical oxidation; DFT

CHE-O2

Theoretical study of the relation between the dressed states and dynamic Stark shift in presence of non-resonant elliptically polarized laser

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Owing to the recent development of laser science and technology, the quantum laser control of ultrafast electron dynamics has been explored actively, and laser-induced π-electron rotations and magnetic fields are expected to establish a principle for the next-generation switching or optoelectronics devices. In the past it was commonly accepted that the coherent π-electron rotation could not be generated in low symmetry aromatic ring molecules, which have no degenerate electronic excited state. Recently we demonstrated that the unidirectional π-electron rotation can be generated even in low symmetry aromatic ring molecules using the two linearly polarized lasers under fixed nuclei [1], and the nuclear vibrational effects are also considered in the adiabatic approximation, where a weak coupling of electron-vibrational interaction is assumed [2].

In this talk we show that a stationary angular momentum is generated even in low-symmetry aromatic ring molecule in the photo-dressed state by introducing the relationship between the Stark shift picture and the dressed state picture. It is found that the dressed states are equivalent to the energy eigen states which are formed by two lasers with same frequencies i.e., elliptically polarized laser, and the difference between two pictures is the initial condition at t=0, that is, in the Stark picture only the ground state is initially populated, on the other hand in the dressed state picture, eigen states which consist of the ground and excited states are initially populated.

Keywords: Dressed state; Elliptically polarized laser; π-electron; Stark shift; aromatic ring molecules;

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CHE-O3

INVESTIGATING AXIAL LIGAND FUNCTIONALIZED 2D COBALT PORPHYRIN MOFS FOR PHOTOCATALYTIC CO_2 REDUCTION: A DFT STUDY

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A search for new photocatalytic materials for the CO_2 reduction reaction has attracted tremendous attention to current research. Two-dimensional (2D) cobalt porphyrin-based organic frameworks (Co-PMOF) has recently been proposed as promising photocatalysts owing to their excellent charge transfer properties and electron-hole separation. In this work, we investigated the structural, electronic properties, and reaction mechanism of CO_2 reduction reaction on the axial ligand functionalized 2D cobalt porphyrin MOFs using the density functional theory method (DFT). Computations reveal that axial ligands play two important roles in enhancing photocatalytic activities of Co-PMOF. (i) It changes the electronic structures of the Co-PMOF leading to reduction of band gap and improves its ability to harvest visible light. (ii) It reduces the potential determining step of CO_2 reduction reaction which in turn hastens the kinetics of the reaction. This study provide insight into the design of high-performance 2D porphyrin MOFs for photocatalytic CO_2 reduction.

Keywords: Photocatalysis; CO_2 Reduction; Cobalt porphyrin MOFs; density functional theory

CHE-O4

INSIGHTS INTO THE OXYGEN EVOLUTION REACTION MECHANISM ON IRON-COBALT-NIKEL-MOLYBDENUM HIGH-ENTROPY ALLOY CATALYSTS: A COMBINED DENSITY FUNCTIONAL THEORY AND MACHINE LEARNING STUDY

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The oxygen evolution reaction (OER) plays a critical role in many energy conversion and storage devices. The development of efficient and stable OER catalysts is of importance for the practical application of these technologies. High-entropy alloys (HEAs) are a class of materials composed of multiple elements in equiatomic or near-equiatomic ratios, which exhibit unique structural and functional properties. In particular, FeCoNiMo-based HEAs have shown promising activity and stability as OER catalysts, but the underlying mechanism of their performance is not well understood due to the vast number of potential active sites on the catalyst surface. In this work, we use a combination of density functional theory (DFT) calculations and machine learning techniques to investigate the OER activity and stability of FeCoNiMo HEA catalysts. By analyzing the electronic structure and adsorption energies of reaction intermediates on the catalyst surface, we identify the most favorable OER active sites and propose design principles for improving the OER activity. Furthermore, we train machine learning models on the DFT data to predict the OER activity and stability of FeCoNiMo HEA catalysts under different reaction conditions. Our findings provide insights into the OER mechanism on HEA catalysts and pave the way for the rational design of efficient and durable OER catalysts based on HEA materials.

Keywords: Oxygen evolution reaction; High-entropy alloys; Density functional theory; Machine learning

CHE-O5

MULTI-SCALE SIMULATION APPROACH FOR STRUCTURE OPTIMIZATION OF DYE-SENSITIZED SOLAR CELL DEVICES

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Features of Dye-Sensitized Solar Cells (DSSC) are low-cost production, wide variety of designs, independence of installation sites, etc. Further improvement of the maximum conversion efficiency is relied on better understanding of the energy conversion mechanisms and precise modeling for design optimization [1].

We firstly reported the development of our original multi-scale DSSC simulator in Ref. 1 and 2, and then have continuously extending the function and predictability of this simulator. This method enables the evaluation of the I-V characteristics for DSSC devices at macro-scale from the nano-scale properties and meso-scale structures of applied materials, which is achieved by integrations of each scale of simulators. The nano-scale simulation reveals physical properties and electronic structure of materials through quantum chemical calculations. The meso-scale simulation consists of the following three simulations: a three-dimensional porous structure simulation to construct a model of the porous TiO_2 electrode, an electron diffusion simulation within the network of TiO_2 particles, and a simulation of tortuosity in the electrolyte. The macro-scale simulation gives the I-V characteristics for DSSC devices using the data from the lower-scale simulations.

In this study, we performed simulations about several mesoporous structures of TiO_2 electrode. The conventional porous structures and novel honeycomb-like structures were constructed, and the characteristics of DSSC based on each TiO_2 structures were estimated by means of a multi-scale simulation. We investigated the difference of the electron diffusivity and their effect on the I-V characteristics, and estimated that highly orderd honeycomb-like structures will be an optimum structure for the electrode of DSSC.

Keywords: Dye-Sensitized Solar Cells (DSSC); Multi-Scale Simulation; Titanium dixide (TiO_2); I-V characteristics; Photoelectrode

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CHE-O6

FIRST–PRINCIPLES STUDY OF SURFACE SEGREGATION ON BIMETALIC CuZn(111) IN PRESENCE OF VARIOUS GAS ADSORBED FOR CARBON–DIOXIDE REDUCTION REACTION (CO_2RR)

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The carbon dioxide reduction reaction (CO_2RR) is an attractive approach for the conversion of carbon dioxide into valuable chemicals and gases. However, the development of efficient and selective CO_2RR catalysts remains a challenge due to the kinetically sluggish nature of the reaction and the complex reaction pathways. CuZn-based catalysts have recently emerged as a promising material for CO_2RR due to their high activity and selectivity towards desired products. Surface segregation of Cu and Zn atoms on the catalyst surface has been suggested to lead to enhanced CO_2RR performance by creating more active sites and modifying the electronic properties of the surface. In this work, we used Density Functional Theory (DFT) calculations to investigate the effect of surface segregation on the catalytic activity of CuZn surfaces towards CO_2RR. Our study focused on the gas-induced surface changes that occur during the reaction, and we found that these changes significantly affect the catalytic activity of the bimetallic surfaces towards CO_2RR. Our results provide insights into the surface chemistry of bimetallic surfaces and their catalytic activity, which can aid in the rational design of efficient bimetallic catalysts. These findings offer new opportunities for the development of more effective CO_2RR catalysts, which are critical for mitigating climate change and transitioning to a sustainable energy economy.

Keywords: Carbon dioxide reduction reaction; Density Functional Theory; Surface segregation; Gas–induce surface change

CHE-O7

MERCURY OXIDATION AND METHYLATION REACTIONS IN NATURAL GAS PROCESSING WITH SOLVATION EFFECTS: A DFT STUDY

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Mercury, a toxic element usually found in the earth's crust, contaminates oil and natural gas. As it has a serious impact on health and ecosystem, more details about mercury reactions in the gas industry are very essential in order to regulate the mercury emissions. However, there are only a few works on the contaminated mercury in natural gas production which always faces these harmful substances. In this article, the abiotic mercury methylation and oxidation reactions, involved the production of some most concerned species such as $(CH_3)_2Hg$, CH_3HgCl, CH_3HgI, and HgI_2 were investigated by Density Functional Theory (DFT) at M062X /DEF2-TZVP, M062X/ LANL2DZ, and B3LYP/LANL2DZ levels of theory. The transition state and activation energy were calculated via Nudged Elastic Band method (NEB). The calculations were integrated with Solvation Model based on Density (SMD) on some solvents of different polarity that are present during the oil-gas transportation and refining processes such as water, toluene, xylene, 1,2-Ethanediol. The simulations were performed under the natural gas environments at controlled temperature 400K. For the reaction (CH3Hg)2S→HgS+(CH3)2Hg, the overall trend of difference of energy between initial and transition state has no significant difference between basis sets which is around 40 to 70 Kcal/mol while enthalpy and vibrational frequency are varying. The solvent effects from toluene and xylene are near to each other and create a slightly higher result than 1,2-Etandiol and water.

Keywords: Mercury oxidation; Abiotic methylation; Natural gas; SMD; DFT

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CHE-O8

THE CATALYTIC ACTIVITY OF SINGLE TRANSITION METAL ATOM DECORATED IN NITROGEN-DOPED GRAPHENE FOR HCOOH DEHYDROGENATION: A DFT STUDY

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The catalytic activity of a single transition metal atom decorated in nitrogen-doped graphene (TM@N_4G; TM = Fe, Co, Ni, Ru, Rh, Pd, Ir, Os, and Pt) for HCOOH FA decomposition has been investigated by using the cluster of TM@N_4G modeled by the Density Functional Theory (DFT) study. Our calculations found that all metals are strongly bound to nitrogen atoms of graphene. Fe@N_4G catalyst provides the strongest binding energy, demonstrating that it is more stable than other ones. The FA dehydrogenation mechanism over Fe@N_4G has been extensively investigated to understand the catalytic efficiency of the Fe@N_4G surfaces. All possible pathways were proposed in two pathways, namely (i) formate and (ii) carboxylate pathways. It occurs through two steps: the first step is the formation of formate (HCOO-) or carboxylate (-COOH) intermediate. The second step is the CO_2 and H_2 formation. The results show that the formate pathway is the most favorable than the carboxylate pathway over the Fe@N_4G surface (HCOOH* $\rightarrow$ HCOO* + H* $\rightarrow$ H_2 + CO_2). The rate-determining step is the C-H bond break to produce CO_2 with an activation barrier of 0.81 eV. Our results will be important for improving the performance of catalysts for the industrially important H_2 production from FA reactions.

Keywords: Nitrogen-doped graphene; Density functional theory (DFT); Formic acid

CHE-O9

RELATIONSHIP BETWEEN THE WATER DISTRIBUTION ON CARBON SUPPORT SURFACE AND PROTON CONDUCTION PATH: LARGE-SCALE REACTIVE MOLECULAR DYNAMICS SIMULATIONS

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Higher output of polymer electrolyte fuel cells (PEFC) is required for many industrial fields. For high electrode reaction activity, optimization of the catalyst layer (CL) structure, which consists of carbon support, ionomer, water, and Pt, is a key factor. The higher-performance CL structures have been investigated by using simulation methods, such as first-principle calculation and differential equations, which can propose theoretical design principles. However, these approaches can not consider the behavior of atoms and large-scale complex CL structures, simultaneously. In a previous study, we successfully optimized the pore size of carbon support with reactive molecular dynamics (RMD) simulations which can consider both chemical reactions and large-scale CL structures [1]. In this work, we focused on the distribution of water which mediates the proton transfer process. Improvement of the wettability of carbon support by the termination of hydroxyl groups to the carbon support surface can alters the water distribution. Therefore, by RMD simulations, we constructed large-scale CL structures of 1 million atoms and investigated the relationship between the water distribution on the carbon support surface and proton conduction to propose the design principles for high-performance cathode CL.

By increasing the ratio of hydroxyl groups on the carbon support surface, the amount of water distributed on the carbon support surface was increased. Furthermore, the amount of water cluster, which can conduct protons, was also increased. These results indicate that higher proton conduction can be achieved by increasing the ratio of hydroxyl groups on the carbon support surface and controlling the water distribution.

Keywords: Polymer electrolyte fuel cell (PEFC); Cathode catalyst layer; Reactive molecular dynamics; Proton conduction; Hydroxyl groups

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CHE-O10

THE DIFFUSION COEFFIECIENT OF MERCURY AND MERCURY COMPOUNDS IN CRUDE OIL AND WATER AT DIFFERENT POSSIBLE TEMPERATURES

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Although a very small amount of mercury is found in crude oil and natural gas, it causes significant harm to their transportation system in both the short and long terms. In the short term, the presence of mercury leads to toxic and contaminated crude oil and natural gas, which requires additional treatment for its removal and therefore increases the production cost. In the long term, its leftovers in the transportation pipeline can cause steel embrittlement, which is one of the major concerns for the pipeline's corrosion. The diffusion of the mercury species in the particular media, such as water and crude oil, determines their possibility of reaching the pipeline's surface and causing the harmful problem. In this work, we mainly focus on the investigation of the transport behavior of mercury species through the self-diffusion coefficient using all-atom molecular dynamics (MDs) simulation. The self-diffusion of mercury species as Hg^0, $(CH_3)_2Hg$, and $(C_2H_5)_2Hg$ in a system of TIP4P water and the crude oil simulated as a mixture of hexane, heptane, octane, nonane, cyclohexane, cycloheptane, toluene, and benzene is determined through the mean square displacement (MSD) at different temperatures, 300 K, 350 K, and 400 K. The simulations have been repeated and analyzed statistically to obtain a reasonable fit for each particular condition. For the result, the MSD tends to be higher in crude oil environment. For instance, the result of mercury in both environments at 350 K is shown below.

Keywords: Molecular dynamics simulation; diffusion coefficient; MSD; mercury; crude oil

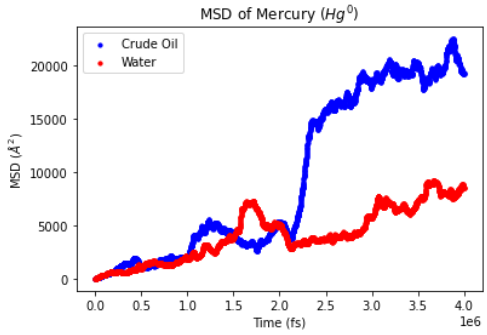

Figure 1. MSD of mercury in crude oil and water environment

CHE-O11

A MOLECULAR DYNAMICS SIMULATIONS STUDY OF GALLIUM MONOLAYER AS A SUPERCAPACITOR APPLICATION

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This study elucidates the performance of the electrode systems, Gallenene a_{100} and b_{010} as an application in supercapacitors using molecular dynamics simulations. The analysis of the radial distribution function (RDF), coordination number, and mean squared displacement (MSD) indicated that Gallenene shows significant potential for improving supercapacitors' energy storage capacity and efficiency. Specifically, Gallenene a_{100} exhibited higher coordination numbers, a larger MSD, and a more well-defined double layer, which are all crucial factors for high-performance supercapacitors. The findings of this study suggest that Gallenene a_{100} is a promising candidate for the development of high-performance supercapacitors. The unique properties of this material make it an attractive alternative to traditional electrode materials like borophene. Further research is needed to explore the practical applications of Gallenene a100 in supercapacitor technology.

Keywords: Gallenene; borophene; molecular dynamics simulations; electrode; supercapacitors

CHE-O12

COMPUTATIONAL SCREENING OF TRANSITION METAL DOPED $MO_2B_2O_2$ AS CATHODE MATERIALS OF LI-SULFUR BATTERIES

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Lithium-sulfur batteries have been proposed as a next-generation energy storage technology owing to their high theoretical energy density. However, they are limited by capacity fading and cycling stability caused by the shuttle effect from soluble lithium polysulfides (LiPSs), and the sluggish decomposition of small LiPSs. In this presentation, I will discuss the design strategy for promising cathode materials based on two-dimensional transition metal boride (MBene), $Mo_2B_2O_2$, using first-principles methods. Various transition metal atom doping as single-atom catalysts (TM-$Mo_2B_2O_2$) was explored to alleviate the shuttle effect and reduce the energy barrier of the delithiation reaction during the charging process. Our computational studies suggest that the presence of TM doping can significantly enhance Li polysulfide (LiPS) adsorption due to the strong formation of TM-S and Li-O bonds, which can help to prevent LiPS dissolution and inhibit the shuttle effect. TM doping can facilitate the delithiation kinetics of small LiPS by reducing the energy barrier. Furthermore, the type of transition metal doping can influence the adsorption energy and reactions in the charging process due to the distinct characteristics of each transition metal atom. In summary, we suggest that all TM-$Mo_2B_2O_2$ is a promising cathode material that can accelerate the reactions of Li-S batteries. Our finding provides useful guidance for the rational design of new MBene cathodes for high-performance Li-S batteries.

Keywords: Lithium-sulfur batteries, Single-atom catalysts, Transition metal borides (MBene), Density functional theory, First-principles method

CHE-O13

CARBON DIOXIDE REDUCTION REACTION ON NON-METAL-DOPED GRAPHITIC CARBON NITRIDE CATALYST: A DFT STUDY

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Excessive use of fossil fuels has led to a rapid increase in carbon dioxide (CO_2) emissions, leading to a series of serious environmental problems, of which global warming is the most urgent. Searching for metal-free catalysts for the CO_2 reduction reaction (CO_2RR) has been a key challenge in the electrosynthesis of fuels for CO_2 utilization. To enhance the catalytic activity of CO_2RR towards C_1 products (CO, HCOOH, CH_3OH, and CH_4), the catalytic role of non-metals (B, P, and S) doped graphitic carbon nitride (g-C_3N_4) materials have been studied by using a density functional theory (DFT) calculation. There are two possible sites for non-metal doping namely substitutional and interstitial. By the way, the substitutional site can be classified into 5 possible sites, including N1, N2, N3, C1, and C2 sites. The results found that the most stable doping site for both B and P atom is substituted at C1 site, while S atom prefers to substitute at N2 site, which corresponds to the lower formation energy. As a result, the most stable site for each B, P, and S-doped g-C_3N_4 surfaces were collected to study the electro-reduction reaction. The results showed that the major product of CO_2RR over B-doped g-C_3N_4 is CH_4, while HCOOH is the major product over P and S-doped g-C_3N_4 surfaces. The limiting potential (U_L) to produce these major products are -0.96 V, -0.73 V, and -0.17 V over B, P and S-doped g-C_3N_4 surfaces, respectively. This theoretical investigation could help design metal-free catalysts for the CO_2RR.

Keywords: DFT; CO_2 reduction reaction; non-metal-doped g-C_3N_4

CHE-O14

ENHANCING THE PERFORMANCE AND STABILITY OF PEROVSKITE SOLAR CELLS THROUGH POTASSIUM HALIDE SURFACE TREATMENT AT THE SNO_2/PEROVSKITE INTERFACE: A COMBINED EXPERIMENTAL AND DENSITY FUNCTIONAL THEORY STUDY

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Interface engineering is essential for improving power conversion efficiency (PCE) and stability of perovskite solar cells (PSCs) by refining the interfacial properties at the interface between carrier transport layers and perovskite to reduce interfacial carrier losses and degradation problems. In this work, we study the effects of adding potassium halide salts (KI, KCl, and $KI_x Cl_{1-x}$) treatments at the SnO_2/perovskite interface using both simulations based on density functional theory and experimental measurements. We aim to understand the mechanism of halide anions and potassium cations in surface defect passivation at the atomistic level. Our research shows that adding halide anions to the interface between SnO_2 and $MAPbI_3$ makes the distortion caused by hydroxyl groups on the surface of SnO_2 much less severe while adding potassium cations stabilizes the contact between SnO_2 and perovskite. This stabilization results in better inhibition of interface degradation and ion migration, better charge transfer properties, and reduced non-radiative recombination, leading to improved PCE and stability of the PSCs. Most importantly, our mixed halide passivation method exhibits superior stability and a better suppression of deep-trap defects and distortion at the SnO_2/$MAPbI_3$ interface. These findings offer new insights into interfacial engineering strategies for enhancing the performance and stability of PSCs.

Keywords: Interface engineering, potassium halide salts, SnO_2/perovskite, stability.

BIO-O1

Enhancing stability and solubility of Piperine by complexation with beta-cyclodextrins: A COMBINED Computational and Experimental STUDY

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Piperine (PP) is a nitrogenous alkaloid found in black pepper, which is known for its poor water solubility. To enhance its solubility and bioactivity, PP can form inclusion complexes with cyclodextrins like β-cyclodextrin (βCD) and its analogs, such as methylated (M), hydroxy-propylated (HP) and sulfobutyl-ether (SBE) βCDs. These cyclodextrins can encapsulate lipophilic guests inside their hydrophobic inner cavity and hydrophilic exterior. In this study, the dynamics and stability of inclusion complexes of PP with βCDs were studied using theoretical and experimental techniques. The results of all-atom molecular dynamics simulation and molecular mechanics/generalized Born/Poisson-Boltzmann surface area (MM/GB(PB)SA) free energy calculations revealed that PP can form complexes with βCD and its analogs in different forms, mainly through van der Waals interactions. Furthermore, the results suggest that the inclusion complex of PP with SBEβCD is the most preferential host molecule, as it has the highest number of atoms in contact and the lowest solvent accessibility inside the hydrophobic cavity, as seen in the ΔG_{bind} ranked in order of PP/SBEβCD (−4kcal/mol) > PP/HPβCD (−4 kcal/mol) > PP/DMβCD (-3 kcal/mol) > PP/βCD (-2 kcal/mol). The A_L-type diagram of the phase solubility studies of PP indicated the formation of inclusion complexes with the 1:1 molar ratio and 576 M^{-1} stability constant at 25°C for SBEβCD. Overall, the findings suggest that inclusion complexes with βCD derivatives, especially SBEβCD, can serve as suitable hosts to encapsulate PP and enhance its solubility.

Keywords: Piperine; β-cyclodextrin derivatives; inclusion complexes; solubility enhancement ; molecular dynamics simulation

BIO-O2

In Silico Studies of Selected Metformin Derivatives Against α-glucosidase and α-amylase as potential antidiabetic drug.

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Type 2 diabetes mellitus (T2DM) has a wide range of symptoms, making it difficult to treat it effectively with a single drug. Long-term metformin therapy for diabetics resulted in a considerably lower risk of stroke incidence or better functional recovery, which was unrelated to the medication's glucose-lowering effects. In this study, a computational framework was applied to discover new potential drugs. Based on previous experimental studies, selected metformin derivatives with a different functional group, Met1, Met2, Met3, and Met8 have been screened and performed molecular dynamics simulations using alpha-glucosidase and alpha-amylase. Autodock Vina and AMBER20 were used for computational studies. Lipinski's rule of five held true across all derivatives and the SWISS ADME online website server was utilized to compute ADME properties of metformin analogues. Clarification of residue interactions between selected metformin derivatives and binding pockets of both enzymes was analyzed and clarified.

BIO-O3

WAVELET ANALYSIS OF INFLUENZA EPIDEMICS ASSOCIATED WITH PM10 AND METEOROLOGICAL FACTORS IN BANGKOK, THAILAND

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Influenza is a respiratory disease caused by influenza viruses and meteorological factors such as temperature, relative humidity, and precipitation play an important role in the transmission and severity of influenza infection. Moreover, air pollution, like particular matter with a diameter of 10 micrometers or less (PM10), can also exacerbate respiratory symptoms and make people more susceptible to infections. Thus, we use the wavelet analysis to study the association between influenza cases and meteorological factors (mean temperature, mean relative humidity, and mean precipitation) including air pollution (PM10 concentration) in Bangkok, Thailand during 2003 - 2019. Wavelet transform of influenza cases shows that there is influenza transmission every 6 and 12 months. Cross-wavelet coherence analysis shows that the annual circulation of influenza dynamics was driven by meteorological factors for the studied period, except in 2005 and 2014. In addition, PM10 was also suggested as a key factor affecting the influenza dynamics over 6 months period. These findings can help us to understand the influenza dynamic pattern and the impact of meteorological factors and PM10 on disease circulation.

Keywords: Wavelet transform; Coherence; Influenza; PM10; Meteorological factors

BIO-O4

MODELING COVID-19 TRANSMISSION IN THAILAND: THE ROLE OF VACCINATION, NPIS, AND TREATMENT

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The global outbreak of COVID-19 has brought the significance of mathematical modeling to the forefront of comprehending the transmission patterns of the virus and devising appropriate public health interventions. This study aimed to explore the transmission dynamics of COVID-19 in Thailand through the development of a compartmental model. Our model incorporates the impact of vaccination and its effectiveness, non-pharmaceutical interventions (NPIs), and treatment in reducing the infectiousness of the population. It classifies the susceptible, exposed, and infected populations into two groups. We fitted our model using real-world data from Thailand, performed a qualitative analysis, investigated the stability of the equilibrium points, and identified the factors that contributed to the asymptotic stability of the corresponding equilibrium points. Additionally, we performed a sensitivity analysis on the basic reproduction number of the model to determine the factors that have the greatest impact on reducing its value. Our results underscore the importance of adapting current public health measures to mitigate the spread of COVID-19. They also highlight the potential utility of mathematical modeling in guiding effective public health strategies to mitigate the impact of pandemics such as COVID-19.

Keywords: Equilibrium points, COVID-19, Stability analysis, Sensitivity analysis, Vaccination, NPIs.

BIO-O5

COMPARATIVE MOLECULAR PROPERTY ANALYSIS ON EBSULFUR AND EBSELEN ANALOGUES AS SARS-COV-2 ANTIVIRALS USING LINEAR REGRESSION AND NON-LINEAR QSAR

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Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) was first reported in Wuhan, China, in December 2019. Even though the number of infected cases has decreased. Discovering novel SARS-CoV-2 antiviral drugs is still interesting for researchers around the world. One of the target enzymes for SARS-CoV-2 is the main protease (M^{Pro}) which is essentially for viral replication. The objective of this study is to find a new compound that has the main protease inhibitory activity of SARS-CoV-2 by using the QSAR technique and molecular docking. The QSAR was used to find the relationship between the structural properties of ebsulfur and ebselen derivatives and the inhibitory activity of M^{Pro}. The ANN model was validated with R^2 and RMSE parameters: R^2 of the training set and test set were 0.89 and 0.10, respectively, and RMSE of the test set was 0.05. The model consists of the shadow length of the Y axis, AlogP98, the shadow area fraction of the YZ plane and the principal moment of inertia Y which are important descriptors that affect inhibitory activity significantly. The model was used to predict the inhibitory activity of thirteen new compounds. Then, all compounds were evaluated for drug-likeness properties and toxicity. Found that P1, P3, P5, P7, P10, P11 and P13 have potential as SARS-CoV-2 M^{Pro} inhibitors and an oral drug. Furthermore, P1 and P7 were more extensively investigated for interactions with molecular docking by VINAXB software. There are interactions with critical catalytic dyads in the active site which are HIS41 and CYS145.

Keywords: QSAR; SARS-CoV-2; Main protease; Ebsulfur; Ebselen

BIO-O6

CYCLICPEPTIFINDER: A DEEP LEARNING APPROACH FOR CYCLIC PEPTIDE DRUG DISCOVERY THROUGH LIGAND PREDICTION

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Cyclic peptides currently play a significant role in drug design and development owing to potentially better specificity to a given target than small-molecule drug and higher membrane permeability than antibody. However, a major challenge for researchers working on cyclic peptide drug development is identifying suitable cyclic peptides for the interesting protein target predicted by *in silico* techniques for using in *in vitro* or *in vivo* studies. In this study, we developed software based on deep learning (DL) algorithms to address these challenges. The software offers two working modes for cyclic peptide construction; (i) the first mode starts with the user inputting cyclic peptide sequence, which is then processed by the DL algorithm to find similar cyclic peptide information, matches potential ligands, scores them, and generates the one-dimensional (1D) cyclic peptide database. (ii) The second mode begins with the user inputting a protein target information. After that, the program will search for the cyclic peptide/protein target-related information by the DL algorithm and subsequentially generates a cyclic peptide database similar to mode (i). Based on these two modes, the generated 1D cyclic peptide database was converted to a 3D structure and performed molecular dynamics optimization. We employed Mean Absolute Error (MAE) as a metric to validate the accuracy and performance of our machine learning model. This program will contribute to developing cyclic peptide-based drugs by streamlining the process and improving efficiency for the docking study.

Keywords: Cyclic peptide; Molecular docking; Deep leaning; Drug design; Peptide modeling

BIO-O7

SCREENING FOR PLANT REGULATORS MODULATING THE EARLY DISEASE-STATE TRANSITION OF CASSAVA BROWN STREAK DISEASE (CBSD) USING DYNAMIC NETWORK BIOMARKER (DNB)

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The sustainability of cassava production is one of the important missions for global food and energy security, especially in Africa and Asia. Cassava brown streak disease (CBSD), caused by the cassava brown streak virus (CBSV), is one of the major factors contributing to significant yield losses up to 70%. Early screening for CBSD detection is an effective strategy to reduce viral spreading and minimize economic losses. Despite several genes associated to CBSV infection were revealed by conventional transcriptome analysis, these differentially expressed genes (DEGs) were often proposed from plants with mild or severe symptoms, leading to the early response genes remaining unidentified. Here, we utilized a Dynamic Network Biomarker (DNB) approach to identify regulators or DNB genes that serve as an early molecular signal of normal-to-disease transition using time series transcriptome datasets of susceptible cassava cultivar under control and CBSV infection condition. The result revealed that 24 DNB genes influenced the normal-to-disease transition at 24 hours after viral infection, before the onset of the CBSD symptoms. The DNB genes mainly consisted of enzymatic genes and transcriptional factors (TFs) participating in various biological processes, such as isoprenoid biosynthetic, photosynthesis, responding to superoxide radicals, and nucleotide biosynthesis. Interestingly, the 3 DNB genes, aminodeoxychorismate lyase (ADC lyase), dUTP-Pyrophosphatase-Like1 (dUTPase), and Hydroxymethylglutaryl-Coa Synthase (HMGS), were hypothesized to be an early defense response for a competition of nucleotide usage between cassava and CBSV which subsequently causes the CBSD. This study provides the potential regulators as early warning signals of CBSV infection in cassava.

Keywords: Cassava; Cassava Brown Streak Virus (CBSV); Cassava Brown Streak Disease (CBSD); Dynamic Network Biomarker (DNB)

HPC-O1

BLOCKCHAIN TECHNOLOGY TO ENHANCE SUPPLY CHAIN MANAGEMENT: CASE STUDY OF COVID-19 ANTIGEN TEST KIT

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Transparency is the primary component of developing trust to ensure the integrity of the supply chain. Each business must provide information and contribute to its supply chain. One of the many products that have been brought out during the pandemic is COVID-19 ATK (Antigen Test Kits) which must be used almost constantly in many situations. In recent years a technology known as blockchain attracted the attention of many individuals. Blockchain is an advanced database mechanism that allocates data within a decentralized system. This paper explores the efficiency of blockchain technology in enhancing supply chain transparency to ensure the quantity of COVID-19 ATK and to simplify the supply chain management experience by using Web 3.0. The proposed system uses smart contracts to record the transaction since the product has been manufactured and transferred across supply chain network. The customer can ensure the integrity of the product by entering the product's details, lot id and expired date, into the blockchain system to query the supply chain history. The work can detect many abnormalizes, such as counterfeit, modified, and smuggle products.

Keywords: Blockchain; Smart contract; Covid-19 ATK; Supply chain management; Web 3.0;

HPC-O2

BLOCKCHAIN TECHNOLOGY FOR HEALTHCARE NETWORKS

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Blockchain is a distributed decentralized database and provides immutability, tamper resistance, and transparency features. Blockchain could be adapted to improve the way they maintain the healthcare data. Blockchain integrated data security and data privacy to establish trust between healthcare network. From our studies, blockchain for healthcare system which explains the relationship between patients and hospitals that were not incorporate further with the insurance part, including indemnity and insurance reimbursement. This work initiated the whole process for receiving treatment at the hospital, from patient registration until payment also included insurance claiming procedure. Another strong point of ours is the privacy policy. Collectively, these allow us to manage the hospital's information systematically in compliance with rules and regulations like PDPA, NHSO, and HIPAA. Careful examination of laws has been conducted to put our project into practice. This work used Hyperledger Besu which is a private blockchain. This system related to the sensitive data, a privacy group and permission are required to prevent unauthorized access. The work describes the technical design for healthcare network and early-stage prototype.

Keywords: Blockchain; Healthcare; Hyperledger Besu; Tessera; Web3;

HPC-O3

COST-SENSITIVE CLOUD ARCHITECTURE FOR AN ONLINE ASSESSMENT WEB APPLICATION

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A university is required to implement online education and evaluation due to the COVID pandemic. The university already has an online learning platform with a fixed resource architecture, but it cannot accommodate the university's examination workload patterns. To address this issue, the university will need to design a new architecture to accommodate the current workload behaviours, as the number of users during the exam will be extremely high, and the workload will spike when students begin taking exams simultaneously. Utilizing a scalable API service and a scalable relational database, this study aims to develop a scalable system capable of handling the increased traffic during exam periods. The evaluation results indicate that the new scalable architecture design can handle the sudden increase in users from zero to five hundred and five hundred to one thousand with an acceptable error rate of 5 percent. However, the expense exceeds the predefined budget of 500 USD monthly, and a scalable relational database is primarily responsible for the high cost. Therefore, we have redesigned the architecture using a hybrid database that is a combination of a relational database with fixed resources and a non-relational database that is scalable and changed the scalable API services from AWS ECS, which requires at least one active instance, to AWS App Runner, which can be configured with zero active instances. This redesign has significantly reduced costs to within the predefined cost while maintaining the reliability and consistency of a relational database and improving the error rate.

Keywords: Auto Scaling; Relational Database; Non-Relational Database; Amazon Web Service

HPC-O4

AGRICULTURAL DATA SHARING TO APPLICATIONS VIA THAGRI

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In today's agricultural sector, data-driven decision making has replaced intuition-based decision making. However, due to a lack of collaboration between data and services, data is not being fully utilized, and various types of data are not being organized efficiently. This deficiently significantly hinders the development of new agricultural application and services. We have design and implement Thailand Agricultural Data Collaboration Platform (THAGRI) to encourage the sharing of agricultural data, which may not be open data. The platform facilitates the exchanges of various types of data including farmland data, soil data, weather data, market locations and growth prediction data, etc. This study aims to develop a platform that enables developers and data providers from both public and private organizations to collaborate and create innovative applications. The platform, called THAGRI, was tested in this preliminary work, and its utility was demonstrated in the creation of several applications, including the Agri-Map, a national agricultural policy tool, the Din-Dee Smart Chatbot, and a crop yield prediction analysis. The results of the study indicate that THAGRI is an effective tool for facilitating the creation of novel applications in the agricultural sector.

Keywords: THAGRI; Agri-Map; data collaboration; data platform; data sharing

HPC-O5

DESIGN AND DEVELOPMENT OF THE BACK-END SYSTEM FOR AN ONLINE LEARNING ASSESSMENT PLATFORM

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The COVID-19 pandemic has significantly impacted people's behavior worldwide, including students and faculty. In order to support the assessment of learning activities during these challenging times, particularly during midterm and final exam weeks when there is a large load on the system and high demand from students, an online learning assessment platform has been proposed. This paper focuses on the design and development of the back-end system for this platform, which is implemented using a RESTful API built with the NodeJS and Typescript frameworks. A cloud architecture has been proposed to ensure that the platform can handle large loads, especially during peak examination periods. This paper describes the first phase of the system design and development process, with a particular focus on the caching technique used to support the retrieval of data with huge loads during critical periods. To manage the variety of information and increase reliability, a non-relational database using DynamoDB has been proposed to handle all information and support caching techniques. The paper also outlines the database design technique used to map information from relational to non-relational databases for data transfer to SQL databases. The user average response time of 500 requests and the Technology Acceptance Model (TAM) was used to evaluate the system's performance and user satisfaction. The evaluation results demonstrate that the system meets all the requirements defined in the first phase, with an acceptable response time.

Keywords: UML diagram; Software requirement; Back-End System; Learning Management System; Technology Acceptance Model;

HPC-O6

A DIVISION ALGORITHM ON MATULA NUMBER SYSTEM

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A non-classical number representation system named Matula number system has been proposed in 1968 by Matula. The concept of two-dimensional model such as tree is used to identify the number. Since the representation in this system is redundant (one number can have more than one representation), we can then simplify the complexity of basic arithmetic operations, especially in multiplication operator. In this work, each natural number can be represented as a rooted tree diagram for Matula representation. We propose, in this work, an algorithm for encoding a representation into our modified Matula code. By utilization of the prime factorization and decomposition of numbers, setting them apart from conventional number systems, we also show that our division algorithm can be performed in $O(n^{3.5})$ where n means the number of nodes in the modified Matula code of the devident.

Classical positional numeral systems represented as strings, which have only a 1-dimensional representation. In this article, we propose an algorithm for performing a division operator on natural numbers represented for Matula codes.

Keywords: Matula numbers; Graphical representation

HPC-O7

INDIRECT SLIDING MODE CONTROL APPLIED TO FAST BATTERY CHARGER OF LIGHT ELECTRIC VEHICLES

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This paper introduced Indirect Sliding Mode Control applied to Fast Battery Charger of Light Electric Vehicles (LEVs). Typically, the battery voltage of an LEV is in the range of 24 to 72 V. Thus, while implementing the single-stage LEVs' chargers, a line- or high-frequency transformer is essentially required. The utilization of a transformer, however, compromises the overall cost, size, and efficiency of LEV chargers. Therefore, a switching mode power supply (SMPS) cascaded with back-end boost converter charger topology is presented in this article, aiming to realize a simple, reliable, efficient, low-cost charger with fast charge properties for the LEVs. The battery used in the test was a Lithium-Ion Phosphate (LiFePo4 32650), size 3.2V, 6.5A/H. The charging circuit is a switching power supply, which reduces the voltage from 220 volts to 12 volts at 40 amperes, and the output is a boots converter to control the charging current to the battery. The results of the experiments demonstrated that closed-loop current charging response is faster than PI control. Besides, the control parameters design is easier than the traditional control system.

Keywords: Fast Battery Charger; Indirect Sliding Mode Control; Light Electric Vehicles (LEVs)

HPC-O8

MODEL AND SIMULATION CURRENT CONTROL OF LED STREET LING BASED ON IBFC CONVERTER OPERATE IN STANDBY MODE

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This paper proposed current control of LED street light driven based on Integrated Boost – Flyback Converter (IBFC) Operate in standby mode. This power state circuit was designed based on the IBFC topologies, which has as main characteristic high voltage gain. Normally, the boost – flyback is designed with the low input voltage application. The advantage of this technique is that use boost converter built up voltage and low current stress of the power switch. A protype single switch was built and operated at 56 kHz fixed switching frequency, 33 V_{DC} output voltage, and 51.48 W output power at the maximum full load. The proposed current control technique achieves regulation current output constancy, which varies level output load from full to Half load and return load condition. simulation result shown good transient response were under/overshoot 0.782 and 3.117 A. Setting time point to 12.81 ms and the return load recovery time to 12.10 ms resulted in set point current approximate 1.56 A. The proposed circuit design was verified via simulation results, which were found to be in agreement with the theoretical analysis.

Keywords: Model; Current Control; Integrated Boost – Flyback; Converter; Standby

HPC-O9

SUGARCANE YIELD PREDICTION BASED ON SATELLITE INDICES AND CLIMATE DATA IN THAILAND

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The sugarcane plant holds significant importance in Thailand's agricultural sector and plays a pivotal role in the country's economy. Apart from its use as a primary source of sugar production, the crop also provides opportunities for the creation of value-added products such as ethanol, biomass electricity, and fertilizers. However, due to the impact of climate change, the output of Thai sugarcane yield is subject to significant variations. In order to mitigate the potential risks stemming from uncertainty, an accurate forecast of sugarcane yield can serve as a valuable guide for farmers, policymakers, and other stakeholders involved in the industry. This foresight allows for informed decision-making regarding the allocation of resources, production planning, and the development of effective market strategies. This study develops a model to predict annual sugarcane yields of 46 sugarcane-producing provinces in Thailand from year 2018 to 2021 by using multiple linear regression. We consider independent variables which are the climate data such as humidity, temperature, precipitation, and growing degree days (GDD), and the satellite data including the normalized difference vegetation index (NDVI). These historical data, obtained from Thailand Agricultural Data Collaboration Platform (THAGRI), are aggregated into each province. In addition, we apply mean absolute percentage error (MAPE) to compare the performance of multiple linear regression (MLR) with or without an additional technique called stepwise selection (SSMLR) and the method of using average values of historical yield as a predictor. Results show that MLR outperforms other models for forecasting annual sugarcane yield of each province from year 2018 to 2021, and the average value of MAPE is 3.97% approximately. By combining statistical techniques, remote sensing, weather data, and sugarcane yield data, this work provides more reliable forecasts of sugarcane yields for each province in Thailand.

Keywords: sugarcane; yield prediction; multiple linear regression; normalized difference vegetation index; stepwise selection

HPC-O10

HYPERMAP GRAMMAR FOR PLANAR K-TREE MAPS

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Engineers and scientists are constantly dealing with increasingly complex models that require suitable mathematical frameworks to describe them. While graphs are commonly used to represent complex systems, maps and hypermaps are more general structures useful for representing and analyzing geometric objects, thanks to additional basic elements that graphs lack, such as faces. In this paper, we propose a novel approach to constructing maps using hypermap grammar. Unlike traditional approaches that rely on vertices and edges to define submaps, our method utilizes vertices and faces to identify and manipulate structures with greater flexibility, since faces play a crucial role in defining maps, especially when they are planar. Our grammar is shown to be effective in both understanding and detecting the structure of the generated maps. We demonstrate how this new grammar can generate planar k-tree maps (where k = 1, 2, or 3) using a single production rule. Our findings suggest that the new hypermap grammar presented in this paper has the potential to be a valuable tool for examining the properties and structure of planar maps, with potential applications in diverse fields such as computer science, topology, and graph theory.

Keywords: Hypermap grammar; Planar maps; Planar k-trees

AIS-O1

STREAMFLOW FORECASTING BY ARTIFICIAL NEURAL NETWORKS IN DIFFERENT CLIMATIC ZONES

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Hydrological simulation is critical in planning and developing a water resource system. Hydrological models are often used to plan, manage, and forecast various variables in the hydrological cycle. In developing nations such as Pakistan, we can modify present prediction approaches and inflow modeling of reservoirs. A suitable approach for forecasting streamflow depends entirely on the data and study region. As a result of decreasing reliance on input data, data-driven solutions are becoming increasingly popular. This study applied various Artificial Neural Network (ANN) models to anticipate daily streamflow, and the results were compared to observed data for a performance evaluation. The research was conducted in regions with different climates: The Garhi Habibullah and Narran. Four Input combinations were used in this study using past daily flow or discharge, precipitation, and maximum and minimum temperature. Statistical measures like Coefficient of determination (R^2), Root Mean Square Error (RMSE), mean square error (MSE), and Normalized root means square error (NRMSE) were used to evaluate the ANN models. General Regression Neural Networks (GRNN) performed well at both stations. At Garhi Habibullah station, the outcomes of statistical evaluation parameters of input combination ($P_A + T_{Amax} + T_{Amin}$) were 0.99, 0.51, 1135, and 5.71 during training, while testing 0.99, 0.00, 0.262, and 0.181 were found respectively. However, at Naran station, the outcomes of these parameters with the input combination ($P_i + T_{imax} + T_{imin}$) were 0.91, 1.23, 20190, and 41.74, while testing 0.96, 0.72, 9247, and 38.90 were found, respectively. Other ANNs models also performed well, but the outcomes of the GRNN model in respect of statistical parameters were more precise.

Keywords: Artificial Intelligence; Neural Networks; Streamflow, Forecasting, Hydrological Simulation

AIS-O2

LAND USE AND LAND COVER PREDICTIONS WITH QGIS-BASED MACHINE LEARNING ALGORITHMS: A CASE STUDY OF THA CHIN RIVER BASIN, THAILAND

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Land use and land cover (LULC) changes have significant impacts on the environment, including water resources, biodiversity, and carbon storage. Accurate prediction of LULC changes is therefore essential for effective land management and environmental planning. The purpose of the study is to illustrate the importance of LULC alterations to the ecosystem. This study presents a case study of the Tha Chin River Basin in Thailand, using Random Forest classification from the Semi-Automatic Classification plugin to classify LULC classes and integrated cellular automata coupled with an Artificial Neural Network (CA-ANN) methodology within the Methods of Land Use Change Evaluation (MOLUSCE) plugin to predict LULC changes in QGIS. To produce land use and land cover (LULC) maps for different time periods, Landsat images from 2000, 2010 and 2020 were analyzed. The classification's performance was evaluated based on various criteria, including overall accuracy and kappa coefficient. The classified 2000 and 2010 maps were used to predict the year 2020. The predicted 2020 map was validated with the classified map. The results gave the accuracy assessment over 80%. The LULC predictions showed a decline in forest cover and an increase in agriculture and urban areas. The study highlights the need of tracking and managing LULC changes in the Tha Chin River Basin and other analogous places while demonstrating the effectiveness of machine learning-based QGIS in properly predicting LULC.

Keywords: LULC change; Random Forest classification; MOLUSCE plugin; SCP plugin; QGIS

AIS-O3

MACHINE LEARNING-BASED COMMUNICATION POWER ADAPTATION FOR CONNECTED TRUCK PLATOONING

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A vehicle-to-vehicle communication (V2V) is a key technology in autonomous and connected vehicles. For a connected vehicle platoon, the communication power utilization is still a key challenge, particularly for long-distance transport. We acknowledge that the historical feedback information from data exchanged within the platoon is advantageous for power optimization. This paper therefore presents a communication power optimization based on Machine Learning (ML) in New Radio (NR) V2V in truck platooning. We performed simulations of the V2V links among truck platooning in the absence of cellular network and infrastructure assistance by a network simulator named MilliCar based on the 3GPP standard. Feedback information among the platoon was also collected for developing the ML models. We compared 3 popular ML classification techniques, namely Random Forest (RF), k-Nearest Neighbors (KNN), and Radial Basis Function Kernel Support Vector Machine (RBF). Afterward, a power adaptation with the optimal ML technique called ML based power adaptation (ML-PA) was proposed. The comparison showed that RF classification technique was slightly better than RBF and KNN for the prediction of transport block reception status of NR-V2V in the platoon. The ML-PA performance was evaluated by comparing with the default power transmission scenario and non-ML power adaptation (PA) scenario. The simulation results indicated that ML-PA developed by RF saved the overall transmitting power in the V2V compared to the default and PA scenarios by 28% and 24% respectively. The ML-PA also reached the maximum power reduction of 56% and 15% while limiting block error rate (BLER) in desired communication range.

Keywords: Platoon; V2V; NR; Power adaptation; Machine learning

AIS-O4

CLASSIFICATION OF SENTINEL-2 IMAGES FOR THAILAND'S PLANTATION DETECTION

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Land use and land cover data are essential for managing large-scale plantations and precision farming. However, traditional survey methods for mapping land use over large areas are expensive in terms of time, labor, and costs. Fortunately, remote sensing techniques have become more robust, sensible, up-to-date, and inexpensive due to technological advances. However, detecting crops, such as rice paddy fields and sugarcane plantations, is a significant challenge for remote sensing. Existing remote sensing methods for identifying plantation areas, such as false color composite and change vector analysis, still have limitations in terms of accuracy. They cannot be widely applied to various regions within the country. Additionally, these methods are only applicable for analyzing data during specific time periods, which means the identification of cultivated areas is only accurate during certain stages of the growing season. Therefore, this study aims to improve a method for detecting these crops using Sentinel-2 satellite images. The study begins with surface reflectance interpretation and noise reduction, then identifies time series surface reflectance value patterns. The process involves supervised learning to differentiate between rice and sugarcane plantations based on their vegetation index change signatures. The results demonstrate that the Long Shot Term Memory (LSTM) method, which uses the Normalized Difference Vegetation Index (NDVI), Normalized Difference Water Index (NDWI), and Normalized Difference Built-up Index (NDBI), can classify rice paddy fields and sugarcane plantations in the testing area with an overall accuracy of 88.13% from the Sentinel-2 images which is high enough for nation-wide agricultural management.

Keywords: Crop Detection; LSTM; Remote Sensing; Satellite Image; Sentinel-2

AIS-O5

DEEP LEARNING FOR COCONUT TREE DECTECTING WITH SATELLITE IMAGERY

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In 2019, Thailand exported fragrant coconuts worth over two billion baht, which was still insufficient to meet the global market demand. Due to the significant demand for coconut products, it is crucial to monitor the cultivation areas periodically to effectively plan and estimate production for processing facilities. Aerial photography can be used to analyze the unique pattern of the perennial coconut plant, and the central coconut-growing region of Ratchaburi in Thailand was selected as the study site for the coconut cultivation areas. To efficiently detect coconut trees in broad areas, modern technology such as Graphics Processing Units (GPUs) can significantly decrease processing time. The You Only Look Once (YOLO) deep learning model was employed to identify coconut trees, and its output was compared with Land Development Department (LDD) data obtained through the THAGRI platform. Our methodology was effective in detecting coconut palms in the region, provided that the trees were not planted too closely together. However, the model's efficiency decreased when the coconut trees were densely planted. In addition to identifying the coconut cultivation site, the YOLO model also identified individual coconut trees, which can significantly decrease the amount of time needed to plan coconut cultivation locations.

Keywords: Coconut; Deep learning; Image processing; Object detection; YOLO

AIS-O6

ONLINE SOC AND SOH ESTIMATION OF LI-ION BATTERY IN ELECTRIC VEHICLES: ARTIFICIAL NEURAL NETWORK

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Li-ion batteries are the most widespread type in the electric vehicle (EV) industry. An expeditious and accurate model for SOC and SOH online estimation is presented in this paper. Since knowing the correct value of SOC and SOH has many advantages, finding the best estimation method is essential. There are several estimation methods. However, the estimation method proposed in this paper considers only the model corresponding to the parameters that are input to the model. Open circuit voltage (OCV), coulomb counting (CC), the conventional methods, are presented in this paper to illustrate their limitations and challenges of them for comparison with a new method. Artificial Neural Network (ANN) is a new method that is expeditious and accurate under specified conditions. The speed is restrictive from calculation time < 36 s, and the accuracy is a mean square error (MSE) < 2%, which the results from the experiment show acceptable results. The ANN model demonstrates high accuracy, speed, and a wide range of working conditions.

Keywords: Li-ion battery; State of charge (SOC); State of health (SOH); Online estimation; Artificial neural network (ANN)

AIS-O7

A PHYSICS-INFORMED NEURAL NETWORK FOR THE DRIFT-DIFFUSION MODEL'S SOLUTIONS TO STUDY SPACE-CHARGE-LIMITED CURRENT DENSITIES IN MILLIMETER-THICK $MAPbBr_3$ PEROVSKITE WITH ION MIGRATION

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Time-dependent drift-diffusion (TD-DD) models governing charge carrier transport are crucial for studying current-voltage characteristics and charge carrier transport properties in a thin-film perovskite device. The traditional methods of solving these models, such as finite difference or finite element that consider spatial and temporal grid points, pose challenges when the thickness of the device is a few micrometers and the time domain is several seconds or minutes. A new grid-less method for solving partial differential equations (PDEs) called physics-informed neural networks (PINNs) has been of great research interest in computational science and engineering. In this study, we use PINNs to solve for coupled, time-dependent, non-steady solutions of the TD-DD model to study the current density characteristics of a single-layer perovskite thin film. This novel method finds the solution by incorporating the PDEs of the TD-DD model as the loss functions in the neural networks. After training a PINN model to minimize the loss functions, including in the initial and boundary conditions, consistent solutions between the electrostatic potential and hole density are obtained. The potential and density gradients are easily computed by using automatic differentiation, such that the current density characteristic is calculated and validated. This work results in an alternative method for solving the TD-DD model in a perovskite thin film that can overcome the challenges of conventional numerical discretization and differentiation.

Keywords: Drift-diffusion; Perovskite thin film; Physics-informed neural networks; Charge carrier; Partial differential equation

CFD-O1

KINETICS MODELING OF TRANSPORT PHENOMENA IN CORROSIVE SYSTEM PIPELINE

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Corrosion is an electrochemical reaction that has an impact on industries, as it can deteriorate materials and equipment used in production processes. It can cause increases in maintenance costs and shorten the lifespan of the equipment. Based on a variety of literature in the fields of physical chemistry to mechanics of fluids, we are aiming to construct a series of models that can effectively yield predictions for the metal loss due to corrosion and under the influence of corrosion inhibitors. The computer modeling begins with inputs for the initial concentrations and diffusion coefficients of species in solution, metal, solution conductivity, and Tafel slopes. The Tafel slopes (β) are extracted from Potentiodynamic polarization curves (PDPs), which can also be used to measure the corrosion potential (E_{corr}) and corrosion current density (j_{corr}) of the system. This is done through the incorporation of mass transport limiting current density to traditional Tafel kinetics. The corrosion measurements of metal loss with the presence of corrosion inhibitors are directly compared with simulated results and validated. The computer model yields new insights into the corrosion prevention mechanism of inhibitors.

Keywords: corrosion; kinetic modeling; electrochemical; Potentiodynamic polarization; transport

CFD-O2

SPECTRAL PROPER ORTHOGONAL DECOMPOSITION OF FLOW PAST CIRCULAR CYLINDER AT SUBCRITICAL REYNOLD'S NUMBER WITH SYNTHETIC JET

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Synthetic jets are frequently used to reduce the drag in flow past bluff bodies. In this wok, synthetic jet is applied to flow past a circular cylinder, which is commonly used to represent flow past the bluff bodies. The flow at $Re \approx 3900$ was simulated using the unsteady Reynolds-averaged Navier–Stokes (URANS) equations with the $k-\omega$ SST turbulent model. The dimensionless frequency of the synthetic jet parameters is defined as 4, while the momentum coefficient is $6.5 \ \ 10^{-3}$. The result shows a 7% reduction in drag and a shift in vortex shedding frequency from 2.05 Hz to 1.526 Hz. The Spectral proper orthogonal decomposition (SPOD) was used to extract the physics of drag reduction. With default parameters of SPOD, it provides 6 peak frequencies. The vortex shedding structure without the jet contains the first and third highest energy frequencies are 1.56 Hz and 3.125 Hz. While the second high energy frequency is 8.125 Hz, it demonstrates the synthetic jet structure. The drag reduction structure is related to the frequencies 4.6875 Hz, 6.5625 Hz and 9.8675 Hz, which show the rolled-up shear layer away from the center line and the lowering in wake region. There is additional structure at 8.906 Hz, which the shedding line spread out from the center line behind the cylinder. This additional frequency obtained from increase the elements of each segment twice from the default.

Keywords: Computational fluid dynamics, URANS, Cylinder flow, Synthetic jet, Spectral proper orthogonal decomposition

CFD-O3

Heat Transfer Analysis of $ZnO+Al_2O_3+TiO_2$/DW Based Ternary Hybrid Nanofluid: A Fractal-Fractional Mode

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Nanofluids are used to achieve maximum thermal performance with the smallest concentration of nanoparticles and stable suspension in conventional fluids. The effectiveness of nanofluids in convection processes is significantly influenced by their increased thermophysical characteristics. However, this technology is not ended here; binary and ternary nanofluids are now used to improve the efficiency of regular fluids. Therefore, this paper aims to analyze the natural convection Newtonian ternary nanofluid flow in a vertical channel. The tri-hybridized nanoparticles of zinc oxide, Aluminum oxide, and titanium di oxide is dissolved in base fluid (distilled water) to form a homogenous suspension. The impact of thermal radiation, joule heating, and viscous dissipation are also assumed. The classical Newtonian ternary nanofluid model has been generalized by using Fractal-fractional derivative (FFD) operator. The generalized model has been discretized by using the Crank Nicolson scheme and then solved by using computational software. To analyze the behavior of fluid flow and heat distribution in fluid, the obtained solution was computed numerically and then plotted in response to different physical parameters. It is noted from the figure that when the volume fraction ϕ reaches to 0.04 (4% of the base fluid), the ternary nanofluid flow shows a significant amount of enhancement in heat transfer rate as compared to binary and unary nanofluid flows. This enhancement in the rate of heat transfer leads to improve the thermophysical characteristics such as viscosity, thermal expansion, and heat capacity etc. of the base fluid.

Keywords: Ternary nanofluid; Distilled water; Joule heating; Viscous dissipation; Fractal fractional derivative; Crank Nicolson scheme.

IEE-O1

OPTIMIZATION OF MUTUAL INDUCTANCE COIL DESIGN FOR WIRELESS POWER TRANSFER USING MATLAB/SIMULINK

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The optimization of mutual inductance coils has become a major issue for wireless power transfer systems, particularly for EV wireless chargers. The high coupling coefficient can be calculated, validated with a FEA program, and measured in terms of the specific shape design. The researcher uses the LCC compensator as a resonant tank for an output stage of a 370VDC/11kW with 400VDC input voltage connected with the transmitter and receiver coil to transfer power via the air in this proposed topology. To validate the overall system, the coils with the optimized mutual inductance design will be tested with MATLAB/Simulink. The simulation results show that the proposed technique can also reduce voltage strain in the resonant tank network.

Keywords: LCC resonant compensator, Wireless Power Transfer; Finite Element Analysis (FEA)

IEE-O2

INVESTIGATION AUTOMATE ALGORITHM FOR FINDING FOCUS AND EXPOSURE OF QUALITY CONTROL SYSTEM IN INDUSTRY

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Typically, while evaluating the operation of an image projector on a quality control system, the resolution test image is projected from the image projector onto the camera's optically sensitive sensor. Then, we employ the obtained image to represent the projector's performance. This test demonstrated that the hardware and software of a camera's ability to determine an image with appropriate brightness and contrast are crucial. In this work, we present an automatic method for modifying the exposure value and adjusting the focus in order to provide an image with the appropriate brightness and contrast. Moreover, we emphasize the speed of the algorithms, which facilitates their deployment in industry or practice. Two pieces make up this study. First, Auto-Exposure (AE) modifies the camera settings in order to produce an image with the appropriate brightness and contrast. Second, the Auto-Focus (AF) portion adjusts the location of the camera or lens so that the focus plane of the image falls on the sensor position of the camera. In both sections, we use the histogram-based and gradient-based approaches, respectively. In essence, we describe a new method that enables the camera to quickly discover the ideal image in terms of brightness and contrast.

Keywords: Automatic focus; Automatic exposure; Quality control system; Algorithms

IEE-O3

A GENERALIZED LIU-STOREY SPECTRAL CONJUGATE GRADIENT METHOD WITH APPLICATIONS IN ROBOT CONTROL AND IMAGE RESTORATION MODELS

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Conjugate gradient (CG) methods are known to be efficient and have less memory requirement for solving smooth nonlinear problems. The formulation of spectral or hybrid CG methods that switch between two or more CG parameters mostly ignores part of the values of the parameters that could have been included. More so, the sufficient descent property of these methods is usually shown via a strategy that assumes a possible exclusion of some function values. In order to relax this assumption, a structured LiuStorey (LS) spectral CG method is presented in this paper. The method generalizes the spectral Fletcher Conjugate Descent (CD) method in its formulation, this feature allows the method to maintains fast convergence feature as well as inherit a good restart property. Therefore, the method is always sufficiently descent without any additional requirement and converge globally via mild considerations. In addition, the method is equally applied in solving robotic and image reconstruction models respectively. Finally, the method is robust compared to some standard algorithms in literature.

Keywords: Unconstrained optimization; spectral conjugate gradient method; sufficient descent criteria; motion control; image recovery.

IEE-O4

IMPROVED NEH ALGORITHM FOR PERMUTAION FLOWSHOP SCHEDULING

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The permutation flowshop scheduling problem involves scheduling a set of jobs on a set of machines, where each job needs to be processed in a specific order on the machines and can be found in many real-world applications where optimizing the order of tasks or jobs on machines or resources is crucial for efficient and cost-effective operations. Makespan is a completion time of the last job at the last machine in given schedule, which is important and commonly used as key optimized objective function. The NEH (Nawaz-Enscore-Ham) algorithm is a well-known constructive heuristic algorithm used to minimize the makespan. The algorithm obtains a first jobs list by ordering all jobs in decreasing of their total processing times and then iteratively inserting current k^{th} job of the list at each position in the previous shortest makespan k-1 scheduled jobs, until all jobs are scheduled. Generating the first jobs list for the NEH algorithm is a critical aspect of the algorithm, and ongoing research challenge. In this study, the first job list generating methods based on the data shape of the processing times, including measures such as mean, standard deviation, skewness, and kurtosis are proposed. Using some Taillard's benchmarks, the proposed linear combinations with three (NEH3T) and four (NEH4T) terms are found outperform the original NEH algorithm, which highlight the importance of considering data shape in the generating of the first job list.

Keywords: Flowshop Scheduling Problem; Constructive Heuristic; NEH-Algorithm; Makespan; Data Shape

IEE-O5

DIFFERENTIAL FLATNESS BASED CONTROL LAW FOR 3-PHASE AC/DC CONVERTER FOR HIGH POWER APPLICATION

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The paper presents a new control law for a power factor correction converter (PFC) developed in the stationary and synchronous reference frames. To achieve this goal, A differential flatness base control law is suggested to accomplish this objective. Using the mathematical model, the voltage and current control loops for the PFC are considered and developed. For determining the control and stability issues in nonlinear systems, analytical algorithms were developed. MATLAB/Simulink was used to develop a software system to validate the suggested control strategy. Additionally, a DC microgrid made up of a grid-connected 380V, 2kVA was used in the simulation network. The converters' simulation results demonstrate great power factor and efficiency. According to the investigation, PFC converters are suitable for use with high power applications.

Keywords: Differential Flatness, Lyapunov Stability, Power Factor Correction Converter, Nonlinear system, Grid connected.

IEE-O6

EXTENDED HAMILTONIAN CONTROL LAW OF MULTIPHASE BOOST CONVERTER FOR FUEL CELL POWER SOURCE IN DC-MICROGRID APPLICATION

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The main objective of this paper is to propose a multiphase boost converter with extended Hamiltonian energy control laws for a proton exchange membrane fuel cell (PEMFC) in DC-microgrid applications. In addition, PEMFCs are particularly well-suited for DC-microgrid applications due to their advantages, such as a stable and reliable power source with low emissions and noise. However, the output voltage generated by PEMFCs is quite low (around 48 V) compared to the DC bus voltage level (around 300 V for EV applications) of the DC microgrid. Hence, a multiphase boost converter can be applied to address these issues. On the other side, the constant power load (CPL) is a critical situation that can cause instability and oscillations in the DC microgrid system. To overcome these issues, the proposed extended Hamiltonian energy control laws are applied. This approach has been proven effective in controlling DC microgrid systems with CPL, ensuring stability and high performance. Finally, the proposed control algorithm of the multiphase boost converter has been investigated through simulations using MATLAB Simulink. The obtained simulation results enable verifying the good performance of the DC microgrid with CPL.

Keywords: Hamiltonian Control Laws; Proton Exchange Membrane Fuel Cell; DC microgrid; Multiphase Boost Converter; Constant Power Load

IEE-O7

DESIGN AND MODELING OF A HAMILTONIAN CONTROL LAW FOR A BIDIRECTIONAL CONVERTER IN DC DISTRIBUTION APPLICATIONS

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This article describes the design and modeling of a Hamiltonian control law for a bidirectional converter in dc distribution applications. In comparison to the typical PI compensation technique for the bidirectional converter, the suggested system offers the advantages of a Hamiltonian control law technique that regulates the voltage bus. A Hamiltonian control law does not require the complex converter modeling. By simulating in MATLAB Simulink, the proposed system confirms the notion. The proposed system consists of three converters, one bidirectional and two buck converters connected on the same distribution bus, all of which are designed for a 24-Volt, 50-Watt DC distribution bus. For the bidirectional converter, the Hamiltonian control law is used. The modeling and practical results show that the Hamiltonian control law technique used in conjunction with a bidirectional converter may significantly regulate the DC distribution bus.

Keywords: Hamiltonian Control Law; Bidirectional Converter; DC Distribution

IEE-O8

HAMILTONIAN CONTROL LAW APPLICATION FOR A BOOST POWER FACTOR CORRECTION CONVERTER

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This article reveals the Hamiltonian control law application for achieving output voltage regulation and power factor correction (PFC) in a single-phase boost converter operating under constant power load (CPL). For the average output voltage regulation, the mathematical average model of the single-phase boost converter is first established. Then, the Hamiltonian control law with integrating terms is applied to the controller design. Therefore, the mathematical average model along with controllers is carried out. For power factor correction, the reference signal of the inductance current is modified by multiplying it with one magnitude absolute signal. To validate and study the performance under various operating conditions, the proposed method is simulated through MATLAB Simulink. The performance assessment of the proposed method in the output voltage regulation, power factor correction, and total harmonic distortion is conducted through simulations under dynamic variations of constant resistive load (CRL), constant current load (CCL), and constant power load (CPL). Based on the simulation, the comparison between the proposed method and the conventional proportional integrating controller can be performed, with regard to various parameters. From the simulation results, it is observed that the performance of the controller achieves robustness.

Keywords: Hamiltonian control law; Boost converter; Power factor correction; Output voltage regulation; Constant power load

IEE-O9

HAMILTONIAN CONTROL LAW APPLICATION FOR CONSTANT CURRENT – CONSTANT VOLTAGE WIRELESS BATTERY CHARGING USING A PRIMARY SIDE BUCK CONVERTER

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This paper aims to apply Hamilton's energy control law to constant current – constant voltage (CC-CV) wireless battery charging using a primary side buck converter. 20 A and 360 V CC-CV are sample Lithium battery charging conditions controlled using a 3.7 kW inductive wireless power transmission main side buck converter. In addition, two load models to be analyzed for this power plant analysis are the step-resistance load and the 50 Ah 360 V Lithium battery. The 3.7 kW Inductive Wireless Power Transmission has been designed for low efficiency. 90% of the time. However, wireless communication keeping the control signal at 80 ms delay, was used for the wireless power transmission system. The CC-CV system conditions, load pattern, inductive wireless power transfer parameters, and feedback signal delay time were determined prior to analysis using Hamilton's energy control.

In the Hamiltonian control law study, the average model of the inductive wireless charging buck converter was presented. Second, the Hamilton control law for inductive wireless chargers has been defined for a system's plant. Third, the Hamilton control law has been expressed for the plant-determined. Next, the Hamilton control law is proved by MATLAB. Then, Hamilton's power control law for constant current - constant voltage wireless battery charging using a primary side buck converter was validated using MATLAB/Simulink. The results show that the Hamilton control law is valid to control the primary side buck converter to control the constant current - constant voltage for wireless battery charging.

Keywords: Hamiltonian Control Laws; Wireless Power Transfer; Battery Charging; Buck Converter; Constant Current – Constant Voltage

IEE-O10

A PORT- CONTROLLED HAMILTONIAN APPROCH BASED ON SPEED/TORQUE CONTROL FOR PERMANENT MAGNET SYNCHRONOUS MOTOR DRIVES

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This paper presents a nonlinear control algorithm based on a port-controlled Hamiltonian approach for controlling a permanent magnet synchronous motor (PMSM) drive. The port-controlled Hamiltonian approach is model-based estimation. Subsequently, the load torque and stator resistance (voltage drops in an inverter and motor) are introduced to be calculated by an asymptotically stable state-observer, which can improve the efficiency of the PMSM drives. In this article, we propose simple solutions to the dynamics and stabilization problems of the nonlinear PMSM drive system. To verify the effectiveness of the proposed control algorithm, a software system is implemented with MATLAB/Simulink. The simulation results show that the proposed control has an excellent control scheme during motor-drive cycles with parameter variations.

Keywords: Digital control, Motor drives, Permanent-magnet synchronous machine (PMSM), Port-Controlled Hamiltonian (PCH), Torque control, Variable speed drives (VSD)

IEE-O11

NON-ISOLATED ONBOARD EV CHARGER CONTROLLER DESIGN BASED ON ADAPTIVE HAMILTONIAN CONTROL LAW

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The growth of the electric vehicles (EVs) market and the inadequacy of EV infrastructure, especially EV charging stations, leads to an increase in charging EVs at home or the workplace. Onboard EV chargers (OBCs) have been installed on electric vehicles to charge batteries which consists of active front-end rectifier (AFE) and bidirectional buck-boost converter (BDC). The trend of increasing power ratings OBCs, the improvement in stability and performance has been interesting. This paper demonstrates non-isolated EV onboard chargers with controller design based on adaptive Hamiltonian control law to approach a robust control system. Finally, the feasibility of the proposed controlled scheme is validated by MATLAB/Simulink with an 11kW non-isolated onboard EV charger. In addition, the performance of the proposed controlled scheme is compared with conventional PI control.

Keywords: Non-isolated onboard EV charger (OBCs), active front-end rectifier (AFE), Hamiltonian control law, The bidirectional buck-boost converter (BDC), Conventional PI control

IEE-O12

MODELLING AND SIMULATION OF PS-MODULATED RESONANT INVERTER BASED ON HAMILTONIAN CONTROL LAW FOR INDUCTION HEATING APPLICATIONS

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The modeling of the phase-shift-modulated voltage-source resonant inverter based on the Hamiltonian control law technique for induction heating applications is presented in this paper. The theoretical analysis of the full-bridge series-resonant inverter for output power control is proposed. To reduce the turn-on switching losses for all load conditions, the inverter is operated above the resonance frequency with the zero-voltage switching (ZVS) with adjustable frequency. In order to reach their goal effectively, the results are verified by computer simulation using a MATLAB/Simulink to confirm the validity of the proposed method through a 1kW laboratory prototype.

Keywords: Hamiltonian Control Law; Full-Bridge Series-Resonant Inverter; Zero-Voltage Switching

IEE-O13

HAMILTONIAN CONTROL LAW FOR FUEL CELL/SUPERCAPACITOR HYBRID SOURCE TO SOLVE CONSTANT POWER LOAD STABILITY ISSUES IN DC MICROGRID

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The new control law of a supercapacitor (SC) based storage device combining a proton exchange membrane fuel cell (PEMFC) as a hybrid power plant is presented in this paper. To realize this goal, a Hamiltonian control law is proposed. The paper deals with the new control algorithm to stabilize FC/SC hybrid system under constant power load CPL stability issue in dc distributed network. To validate the proposed control approach, a software system is implemented with a MATLAB/Simulink. Also, the dc microgrid used in simulation network consists of a PEMFC of 2500 W, 50 V and a supercapacitor module of 188.88F 51.3V. The simulation results show that the proposed controller has excellent control performance during a load-drive cycles.

Keywords: DC microgrid, Fuel Cell (FC), Hamiltonian Function, Hybrid Power Source, Lyapunov Stability, Supercapacitors.

POSTER PRESENTATION ABSTRACTS

PHQ-P1

A NOVEL SUPPORT VECTOR MACHINE WITH GENERALIZED PINBALL LOSS FOR UNCERTAIN DATA CLASSIFICATION

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In this study, we have developed a low-cost super-resolution fluorescence microscopy setup that can be used to improve localization precision in single particle tracking. To reduce the cost of the setup, we sourced different components from multiple suppliers, while still maintaining high specifications. Our setup consists of an excitation laser, optic lens and mirror, objective, a CMOS camera, and fluorescent dye. We used custom particle-tracking simulations developed in MATLAB to study the optical parameters of each apparatus part and obtain the localization precision by determining the deviation of the tracked position from the fluorescence centroid. We estimated the diffusion coefficient of mobilizing particles using the mean-squared displacement method or the velocity autocorrelation function. Our simulation results demonstrate that by adjusting the quantum yield, fluorescence intensity, emission rate, and camera gain, the proposed low-cost microscope can achieve a localization uncertainty of less than 10 nm, making it practical for tracking a fluorescent single molecule. The proposed cost-effective setup has the potential to make single particle tracking accessible to a wider range of researchers, as the high cost of super-resolution microscopy is often a limiting factor. Our study offers a valuable contribution to the field of microscopy, providing a more affordable and accessible solution for researchers who require high localization precision in their experiments.

Keywords: Super-resolution fluorescence microscopy; Single particle tracking; Localization precision

PHQ-P2

FABRICATION OF THREE-DIMENSIONAL POLYMER FIBROUS SCAFFOLDS CONTAINING GRAPHENE OXIDE

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Three-dimensional (3D) electrospinning is a technique that uses electrical charges to draw a scaffold from a polymer solution, allowing scaffolds to be fabricated in a 3D shape. This research aims to investigate and identify a new polymer solution and appropriate parameters that can fabricate 3D polymer fibrous scaffolds that are as similar as possible to the original shape. The 3D electrospinning method involves using modified 3D printing to print scaffolds from the positive electrode-connected needle (printed into the negative electrode-connected base) and a syringe that contains the polymer solution and graphene oxide additive. Graphene oxide is used as an additive because this carbon-based nanomaterial can enhance the mechanical and biological properties of the 3D scaffolds. This research uses five different types of graphene as additives and classifies each type of graphene in the 3D polymer scaffolds using SEM, XRD, FTIR, and Raman characterization. The research also fabricates 3D scaffolds without additives for comparison. Additionally, polymer scaffolds fabricated using 3D electrospinning techniques will be characterized and compared using mechanical testing machines and the characterizations mentioned above.

Keywords: 3D electrospining; graphene; polycaprolactone

PHQ-P3

FAST ION ORBIT CLASSIFICATION IN THAILAND TOKAMAK-1 USING SUPPORT VECTOR MACHINE

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The Thailand Tokamak-1 (TT-1) is a small tokamak initially operated with hydrogen plasma in Ohmic mode. Subsequent operations involve equipping the device with auxiliary heating systems, such as neutral beam injection (NBI) or ion cyclotron heating (ICH), which promote fast ions with complex trajectories due to the nonuniform magnetic field of the device. This work presents a computational study of fast ion orbit classification in TT-1 using Support Vector Machine (SVM) algorithms. Accurate classification of fast ion orbits is crucial for optimizing tokamak performance. In this study, we use SVM to classify the complex trajectories of fast ions excited by NBI and ICH heating in TT-1 plasma. Our results demonstrate that SVM accurately classifies fast ion orbits, achieving high accuracy across a wide range of plasma conditions. The ability to accurately classify fast ion orbits has important implications for optimizing tokamak performance and improving the efficiency of fusion reactions. This also highlights the potential of the SVM algorithm for analyzing complex data in plasma and nuclear fusion research.

Keywords: Thailand Tokamak-1; Fast Ions; Support Vector Machine; Orbit Classification; Plasma

CHE-P1

A DFT STUDY ON A SINGLE TRANSITION METAL DOPED C_3N FOR CO OXIDATION REACTION

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Carbon monoxide (CO) is one of the major common toxic gases in the atmosphere, originating from car exhausts, industrial processes and incomplete burning of fuels or petroleum products. The catalytic oxidation of carbon monoxide (CO) by oxygen (O_2) molecule is one of the most popular methods for conversion of CO to the less toxic molecules, i.e., CO_2. The C_3N monolayer is an interesting catalyst for CO oxidation reactions due to its unique electronic and structural properties as well as high surface area. In this work, we investigated the adsorption of CO and O_2 molecules on transition metals (TM = Cu, Ni, Pt and Pd) decorated on the single (Cv and Nv) and double vacancy (CCv and CNv) of C_3N monolayer using density functional theory (DFT) calculation. The results show that O_2 is more feasibly adsorbed on N vacancy of C_3N (Nv-C_3N) than CO molecule. Moreover, it is found that the gas adsorptions on Pt@Nv-C3N surface with adsorption energies (E_{ads}) of -3.07 eV are more stable than Cu, Ni and Pd with adsorption energies (E_{ads}) of -1.91, -2.58 and -2.48 eV respectively. In addition, the CO oxidation on Pt@Nv-C_3N monolayer preferentially proceed via ER mechanism rather than that LH mechanism with the rate-limiting step of 0.41 eV as illustrated in Figure 1. By comparison, we found that Pt@Nv-C_3N is predicted to be a potential material for CO oxidation among of these materials. Therefore, we hope that Pt@Nv-C_3N might be a high-performance catalytic material for highly effective material for CO oxidation reaction.

Keywords: CO oxidation; density functional theory (DFT); transition metal; ER mechanism; LH mechanism

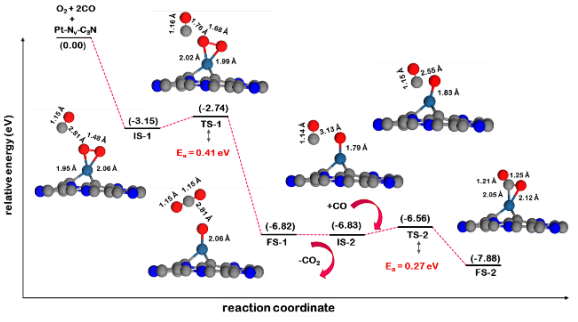

Figure 1. The potential energy profile and optimized stationary points for the oxidation of CO via the ER mechanism.

CHE-P3

HIGHLY SELECTIVE ALUMINUM (III) FLUORESCENT SENSOR AND DFT SUPPORT ALUMINUM SENSING MECHANISM

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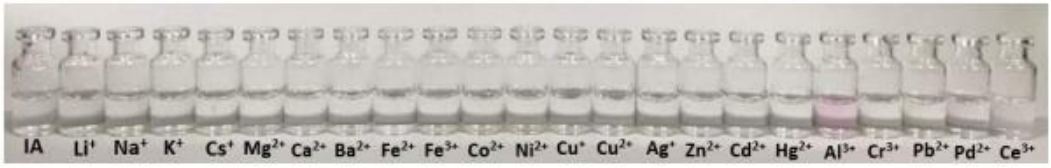
The design and synthesis of a novel bis(rhodamine)-based fluorescent sensor, IA, for the detection of Al^{3+} ions have been accomplished. The IA probe was designed with two rhodamine groups connected by 2,5-thiophene dicarboxylic acid in the expectation of enhancing fluorescence and sensing Al^{3+} rather than other metal ions. In a 2:1 CH_3CN-H_2O (v/v) solution, the IA probe changed from colorless to pink upon the addition of Al^{3+} and exhibited a significant fluorescence enhancement. Job's plot analysis confirmed the 1:1 stoichiometric structure of IA and Al^{3+}. The detection limit (LOD) of Al^{3+} was calculated to be 76.3 pM, a level sufficient for detecting Al^{3+} on the picomolar scale with a linear range of 0-80 μM . In addition, density functional theory (DFT) calculations were performed on IA-Al^{3+} complex to further support the plausible Al^{3+} sensing mechanism.



Keywords: Density functional theory (DFT); Metal support interaction; Rhodamine; Detection of Al^{3+} ; Fluorescent chemosensors

CHE-P4

ADSORPTOIN OF METALS FROM E-WASTE ON CHITOSAN AND CHITOSAN/GRAPHENE OXIDE COMPOSITES: INSIGHTS FROM DFT CALCULATIONS

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The adsorption interactions between metals on chitosan (CS) and chitosan/graphene oxide composites (CS/GO) were investigated by density functional theory (DFT) at the B3LYP level with 6-31G(d,p) and LANL2DZ basis set. The effect of water as solvent was included using the polarizable continuum model (PCM). Tl^{+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Sr^{2+}, Cd^{2+}, Ba^{2+}, Pb^{2+}, Cr^{3+}, Ge^{4+}, and Te^{4+} have been selected as the metals to be studied because of high impact in electronic waste (E-waste). Model structures, adsorption energy, HOMO-LUMO calculations, and molecular electrostatic potential (MEP) are necessary to predict the formation of complexes. The interaction between CS and CS/GO and metal species was shown in almost all cases as covalent partial. In addition, all CS-metal and CS/GO-metal complexes were placed close to the nitrogen atom were shown to be stronger than oxygen atoms, because the charge density of the nitrogen is increased in the formation of the Schiff base with the proximity of the aromatic rings. The HOMO and LUMO energy gap were decreased when the CS and CS/GO binding with the metals. The interaction between CS/GO showed more selectivity for metals than CS. Finally, the chitosan and chitosan/graphene oxide composites have stability in water and is therefore considered as a material in the field of processing of E-waste and environmental pollution.

Keywords: Chitosan; Graphene oxide; Electronic waste (E-waste); Density functional theory (DFT)

CHE-P5

THE EFFECT OF SINGLE AND DUAL HETEROATOMS DOPED DIAMOND FOR CARBON DIOXIDE REDUCTION REACTION: DFT STUDY

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The electrochemical reduction of CO_2 into value-added chemicals and fuels holds great promise for environmental problems. Recently, the doping of diamond have attracted much attention in electrochemistry, where surface structure and electronic states play an important role. In this work, we used the Density functional Theory (DFT) to investigate the CO2RR activity of single and dual heteroatoms of boron (B), nitrogen (N), and phosphorous (P) atoms anchored on diamond as a catalyst. Our calculation found that the dual dopant showed an excellent performance for CO2RR when compared with single dopant. In the case of BB and NN, the main product is CH_2O with overpotential of 0.49 and 0.17 V, respectively. For B and N co-doped catalyst (BN), it can be produced CH_2O and HCOOH as a major product with no applied any overpotentials. Moreover, BN is the top of the volcano plot, with the lowest limiting potential (U_L) and also shows excellent thermal stability and ability to suppress the competing hydrogen evolution reaction (HER). This work provides insight into experimental and theoretical studies on the electroreduction of CO_2.

Keywords: Diamond; dual-heteroatoms-doped diamond CO2RR; DFT

CHE-P6

DEVELOPMENT OF HIGH CATALYTIC PERFORMAMCE OF CU-SINGLE ATOMS SUPPORTED ON GRAPHITIC CARBON NITRIDE FOR CARBON DIOXIDE CONVERSION TO VALUE-ADDED PRODUCT: A DFT STUDY

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Carbon dioxide (CO_2) is the one of harmful greenhouse gases that emits from engine of vehicles and industry. The enhancing of atmospheric CO_2 gases resulting in global warming effect. The hydrogenation of carbon dioxide to formic acid ($CO_2 + H_2 \rightarrow HCOOH$) is an important reaction which can both reduce the greenhouse gases and produce useful value-added compound. In this work, the mechanism of CO_2 hydrogenation over the single-atom catalysts (SACs) supported on graphitic carbon nitride (g-C_3N_4) have been investigated by means of Density functional Theory (DFT). The SACs catalyst is composed of Cu atom and g-C_3N_4 monolayer material. Firstly, the adsorption of CO_2, H_2 molecule, and co-adsorption complex (Co-Ads) were calculated. Our calculations found that adsorption energies of CO_2, H_2 and Co-Ads are calculated to be −0.35, −0.31, −0.36 eV, respectively. Moreover, Co-Ads can be adsorbed on Cu-g-C_3N_4 catalysts which implying that CO_2 hydrogenation can be occurred by Co-adsorption pathway via two important intermediates, namely (*i*) formate (HCOO) and (*ii*) carboxylate (COOH). According to DFT calculation, it was found that HCOOH formation can be produced via HCOO intermediate. The hydrogen dissociation step is the rate determining step with activation barrier of 0.64 eV. This work could be provided a more understanding of CO_2 conversion and the future applicability of Cu-g-C_3N_4 catalysts.

Keywords: Single-atom catalysts; graphitic carbon nitride; formic acid; CO_2 hydrogenation; DFT

CHE-P7

COMPUTATIONAL SCREENING OF DOUBLE-ATOMS CATALYSTS DECORATED ON DEFECTIVE BORON NITRIDE FOR CATALYZING CO OXIDATION: A DFT STUDY

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Carbon monoxide (CO) is an environmental pollutant and is harmful to human health. Therefore, CO conversion plays a vital role in solving environmental issues. CO oxidation is the most effective method for converting CO to carbon dioxide (CO_2) in heterogeneous catalysis. In this work, we systematically studied the dual-metals atoms (TM_2 = Mn, Fe, Co, Ni, Cu, Pd, Ag, Pt, and Au) decorated on defective boron nitride (BN) by applying density functional theory (DFT) calculations. We modeled three different configurations of defective BN via the boron-boron vacancy (V_{BB}), nitrogen-nitrogen vacancy (V_{NN}), and boron-nitrogen vacancy (V_{BN}). Dual-metals atoms' stability and structural properties on defective BN are investigated. The calculation results revealed that dual TM atom anchored defective BN is stable and prevents the aggregation of metal clusters on the substrate. Interestingly, all dual TM atoms decorated on BNV_{BB} are more durable than the others. Consequently, we consider the adsorption ability of CO, O_2, and CO_2 on $TM_2@BNV_{BB}$ to screen the suitable catalyst for CO oxidation. We found that Ag, Pd, and Ni atoms appeared the superior performance for this task due to the difference in adsorption energy between O_2 and CO on $Ag_2@BNV_{BB}$, $Pd_2@BNV_{BB}$, and $Ni_2@BNV_{BB}$ is smaller than that of the other. We predicted that $Ag_2@BNV_{BB}$, $Pd_2@BNV_{BB}$, and $Ni_2@BNV_{BB}$ have the best catalytic performance for CO oxidation. Our calculations provide an insight into the details of TMs' stability on defective boron nitride and guide a way to select a suitable catalyst for the CO oxidation reaction.

Keywords: Double atom catalysts; CO oxidation; Density functional theory; Boron nitride; Transition metal

BIO-P1

ELUCIDATING THE MECHANISM OF CALCIUM CARBONATE FORMATION IN THE CARBONIC ANHYDRASE N66 OF *PINCTADA MAXIMA*

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N66 matrix protein (N66) is a 66 kDa sized protein present in the nacreous and prismatic layers of the *Pinctada maxima*, which is often used in the pearl industry. It is a carbonic anhydrase that catalyzes the reaction that converts carbon dioxide and water to bicarbonate and hydrogen ions, with zinc in the active site. This protein contains a very long GN repeat region, similar to the G-X-N repeat region of nacrein (where X corresponds to D or E) in *Pinctada fucata.* The repeat region is a fully disordered structure, which plays an important role in the growth and regulation of calcium carbonate. However, the GN repeat region in N66 is less acidic than nacrein. The function and the mechanism of calcium carbonate crystallization of N66 protein are not fully understood. In this study, we performed theoretical calculations using multiple molecular dynamics simulations to understand how the GN repeat region of N66 contributes to calcium carbonate formation and its detailed structure and function. Our results show that the GN repeat region, confirmed as an IDR region, has less activity in binding carbonate and calcium ions compared to nacrein.

Keywords: N66; molecular dynamics; carbonic anhydrase; biomineralization; nacre

BIO-P2

ENHANCED SOLUBILITY OF 8-BROMOBAICALEIN THROUGH INCLUSION COMPLEXATION WITH β-CYCLODEXTRINS

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Baicalein (5,6,7-trihydroxyflavone), an active compound found in the traditional medicine Scutellaria baicalensis Georgi, has demonstrated anti-inflammatory, antiviral, and anticancer properties. 8-bromobaicalein (BB), a derivative of baicalein, has shown even stronger cytotoxic activity, but is limited by low water solubility. Cyclodextrins (CDs), cyclic oligosaccharides with a hydrophilic outer surface and hydrophobic central cavity, have been used in the pharmaceutical industry as complexing agents to enhance drug solubility and bioavailability. In this study, βCD and its derivatives (DMβCD, HPβCD, and SEBβCD) were investigated for their ability to enhance the solubility of BB through inclusion complexation. Molecular dynamics simulations and MM/GBSA-based binding free energy results indicated that DMβCD was the most effective host molecule for BB inclusion complexation.

Keywords: 8-bromobaicalein; Cyclodextrins; Inclusion complexation; Molecular dynamics

BIO-P3

CISPLATIN LOADED CALCIUM CITRATE NANOPARTICLES AND THE QUANTUM MECHANICAL FOR LUNG CANCER TARGETED THERAPY

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Bronchogenic carcinoma or lung cancer caused most of the cancer death patients with an estimated 1.8 million death (18 %) and the number two most diagnosed cancer with an estimated 11.4% new cases worldwide. Chemotherapy by using anti-cancer drugs is the main therapeutic for lung cancer. However, the limitation is the degradation of drugs and side effects caused by lacking target sites. The nano-biomedical technology attended to the development of targeted therapy. In the present study, cisplatin loaded calcium citrate nanoparticles (CaCit@CDDP NPs) were synthesized by a bottom-up process with the coprecipitation method. Epidermal growth factor (EGF), a specific protein-ligand to epidermal growth factor receptor (EGFR) which is a receptor mostly expressed in cancer cells was applied to be a targeting molecule in synthesized nanoparticles (CaCit@CDDP-EGF NPs). The results found that the CaCit@CDDP-EGF NPs were in the range of 250-350 nm (320.90±23.20 nm), positive zeta potential (+19.75±2.87 mV) with drug loading efficiency and stability. The IC_{50} and cell viability show inhibition of lung carcinoma cells (A549 and H1975) with lower cytotoxicity to normal cell line (MRC-5) compared with cisplatin. For the theoretical study, quantum mechanics (QM) calculations with the DFT method at B3LYP level of theory were performed to investigate the geometry parameters and electronic properties of CaCit@CDDP. The results demonstrated that the binding energy of cisplatin-citrate complexes were in a range of -8.10 to -4.51 eV, supporting the formation of the cisplatin loaded nanoparticles and the stability of nano-drug. The success of synthesized nanoparticles will provide opportunities for novel nanomedicine, information on cisplatin loaded nanocarriers and lung cancer therapeutic.

Keywords: Bronchogenic carcinoma; Calcium citrate nanoparticles; Cisplatin; Epidermal growth factor protein; Quantum mechanics

BIO-P4

Molecular Dynamics Simulation of Isobutylamido Thiazolyl Resorcinol (Thiamidol™) in complex with Human and Mushroom Tyrosinases

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Tyrosinase is an enzyme that plays an important role in the synthesis of melanin and is a viable target for decreasing hyperpigmentation. While several tyrosinase inhibitors have been developed, the majority of them lack clinical efficacy because they were designed based on mushroom tyrosinase as the target. A previous study found that isobutylamido thiazolyl resorcinol (Thiamidol™) inhibits human tyrosinase more effectively than mushroom tyrosinase. Herein, various molecular modeling techniques, including molecular docking, molecular dynamics simulation, and free energy calculation based on the molecular mechanics/Poisson-Boltzmann surface area method, were used to investigate the molecular interactions between Thiamidol™ and human/mushroom tyrosinase at the atomic level. Results indicated that the resorcinol part of Thiamidol™ was located within the catalytic copper center of both human and mushroom tyrosinases, interacted with several residues, including H180, H202, H211, F386, and H390 in human tyrosinase, and F264 in mushroom tyrosinase, primarily through van der Waals interactions. The Thiamidol™/mushroom tyrosinase complex had greater number of destabilizing residues than the Thiamidol™/human tyrosinase system, which was supported by a lower binding affinity of Thiamidol™ for mushroom tyrosinase, as well as increased water accessibility and fewer atomic contacts at the active site of mushroom tyrosinase. Overall, the data obtained from this research may be beneficial for the development of novel tyrosinase inhibitors.

Keywords: Tyrosinase inhibitor; Molecular docking; Molecular dynamics simulation; Melanogenesis; Molecular interaction.

BIO-P5

N501Y MUTATION IN SARS-COV-2 SPIKE RBD PROTEIN ENHANCES ITS BINDING TO ACE2 RECEPTOR

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Studies have indicated that the N501Y mutation in the spike protein of SARS-CoV-2 enhances the binding efficiency between its receptor-binding domain (RBD) and the human angiotensin-converting enzyme 2 (ACE2) receptor, decreasing vaccine effectiveness and increasing the potential for viral infection. In this work, the structures of the wild-type RBD and N501Y-RBD in complex with the ACE2 receptor were generated to evaluate the effect of the N501Y mutation on their binding efficiency using molecular dynamics simulations, free energy calculations based on the MM/GB(PB)SA and SIE methods, and residue interaction network analysis. The results revealed that the N501Y-RBD/ACE2 complex displays higher compactness than the wild-type RBD/ACE2 structure via strong H-bonding, π–π, and van der Waals interactions. Moreover, the number of hot-spot residues in N501Y-RBD/ACE2 was higher than that of the wild-type RBD/ACE2 system. Structural and energetic insights gained from the study could be utilised for the design of novel drugs and vaccines against newly emerging coronavirus strains.

Keywords: SARS-CoV-2, S protein RBD–ACE2 binding, N501Y mutation, MD simulation, residue interaction network analysis

BIO-P6

IN SILICO SCREENING OF PHYTOCHEMICAL COMPOUNDS AGAINST PAPAIN-LIKE PROTEASE ENZYME OF CORONAVIRUS 2019

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The global pandemic of coronavirus 2019 (COVID-19), caused by severe acute respiratory syndrome 2 (SARS-CoV-2) in December 2019 has affected the global economy and industry. In January 2023, there were 600 million cases of infection and 6.6 million fatalities across the globe due to SARS-CoV-2. Therefore, it is urgent need to search for drugs against SARS-CoV-2. Papain-like protease (PLpro) is essential for viral polyprotein cleavage and innate host immune response; hence, it is regarded as an important target for the development of SARS-CoV-2 inhibitors. In this study, various computational tools were applied to find the potential compounds against PLpro of SARS-CoV-2. The obtained compounds were further studied in terms of their roles to stabilize the protein structure as well as protein-ligand interactions. Detailed information can be useful for further designing of PLpro inhibitors.

Keywords: Papain-like protease; SARS-CoV-2; Drug-likeness properties; Molecular docking; Molecular dynamics simulation

BIO-P7

TRANSCRIPTOME STUDY INFERRING DIFFERENT METABOLISMS IN DEVELOPING STORAGE ROOTS OF LOW- AND HIGH-CYANIDE CONTAINING CASSAVA VARIETIES

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Low-cyanide containing (sweet) cassava varieties have a growing demand in food industries, especially for functional food market such as gluten-free flour. In contrast to the demand, cassava root production of the sweet cassava varieties is always low, not only from their growth characteristics but also being susceptible to the prevailing stresses. Here, transcriptome analysis was conducted to decipher the biological molecular mechanism involving in storage root (SR) initiation of sweet cassava cultivars. The early developing SR (~ 40 days after planting (DAP)) of Hanatee (HN), a low-cyanide variety was examined with respect to Kasetsart 50 (KU50), a high-cyanide variety. The results of RNA-seq data analysis were 48 differentially expressed genes (DEGs) with up-regulated in KU50 and 97 DEGs with up-regulated in HN. Based on pathway enrichment analysis of DEGs, MAPK signaling pathway, nitrogen metabolism, plant hormone signal transduction and plant-pathogen interaction were dominant in HN, while metabolic functions of KU50 related to 2-oxocarboxylic acid metabolism, alpha-linolenic acid metabolism, ascorbate and aldarate metabolism, cyanoamino acid metabolism, diterpenoid biosynthesis, fructose and mannose metabolism, glucosinolate biosynthesis, linoleic acid metabolism. These suggested the prominent of secondary metabolite metabolisms in KU50 at SR initiation which supported SR formation. The proposed metabolic processes and related genes may be useful for further investigation in their transcriptional regulation leading to yield improvement of sweet cassava varieties.

Keywords: Cassava; Low-cyanide cultivars; Transcriptome analysis; Storage root development

AIS-P1

IDENTIFYING HUMAN FINGERPRINTS BY USING OPTICAL COHERENCE TOMOGRAPHY IMAGES WITH DEEP LEARNING

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Optical coherence tomography (OCT) has been utilized to generate depth images of living tissue in various fields. In this research, we propose a novel approach to improve the security and performance of traditional fingerprint scanners using OCT technology for internal finger biometrics. Our system utilizes the internal structure of the fingertip, such as sweat glands, epidermis, and dermis, to construct a 3D model of the finger. We extract features from the internal fingertip image using pre-trained deep learning models, including Inceptionv3, VGG16, Xception, ResNet50, and a custom model. A voting method is employed to ensure the system's robustness. We collected a dataset of internal fingertips from twelve unique fingers, representing twelve users, around 1,000 images for each finger. We split 60% of the data for training and the rest for validation. Our experimental results show that the proposed method achieves an accuracy and prediction rate of approximately 99%, as evaluated using the confusion matrix. These results suggest that deep learning-based security systems utilizing internal fingertip data may be able to replace traditional verification systems with higher security. However, the effectiveness of the proposed method must be further validated and tested in real-world scenarios. Additionally, future work may include the integration of this technology with in-house OCT hardware for better practical application.

Keywords: Convolutional neural networks; Optical coherence tomography; Voting method.

IEE-P1

EFFECTS OF DRONE SPRAY PARAMETERS ON DROPLET COVERAGE IN DURIAN CANOPY

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Thailand is the largest grower and exporter of fruit and is an important supplier of both fresh and frozen durian. As a result of its high export value, durian is also known as Chanthaburi's highest-earning fruit crop. In Thailand, most chemicals are sprayed on farms with a hand sprayer, which is not only inefficient and wastes a lot of chemicals, but also makes the health and safety of farmers at risk. Therefore, drones have the advantages of great efficiency and flexibility in solving challenges. However, the impacts of drone spray settings on droplet distribution on durian canopy have not been observed. Spray trials with two parameters (flight height, and flight velocity) and two parts of durian trees (top surface of a leaf and under side of a leaf) are undertaken in this study. Analyzing sprayer droplet images will determine the optimal drone spraying solution for durian trees. SnapCard is a smartphone app that evaluates spray treatments on water-sensitive paper (WSP). The understanding of the relationship between fight parameters and droplet coverage will be made possible by the use of SnapCard and image processing techniques.

Keywords: Drone; SnapCard; Droplet Coverage; Durian

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