

PROGRAM ACS GII + ICCST7 (<https://7thiccst2023.com/>)

8 <sup>th</sup> DECEMBER 2023 (FRIDAY) Pre-Conference Workshop QM MM MD ML AI		
8.00 - 8.30	<b>Workshop Registration / Overview</b> Assoc. Prof. Dr. Vannajan S. Lee <i>Quantum Information Science and Technology (QIST), UMCompChem, MolDesign, Universiti Malaya, Malaysia</i>	<b>UM Computational Chemistry Lab</b> <b>BMK FD-L3-11</b> (New Chemistry Building)  <b>Compchem.um.edu.my</b>
8.30 - 9.45	<b>Quantum Calculation</b> Dr. Tang Wai Kit <i>Quantum Information Science and Technology (QIST), UMCompChem, MolDesign, Universiti Malaya, Malaysia</i>	
9.45 - 10.00	Break	
10.00 - 12.30	<b>Molecular Dynamics</b> Assoc. Prof. Dr. Thanyada Rungrotmongkol <i>Chulalongkorn University, Thailand</i>	
12.30 - 13.30	Lunch / Friday Prayer	
13.30 - 15.45	<b>Machine Learning and Artificial Intelligence</b> Assoc. Prof. Dr. Shirley Siu <i>Macao Polytechnic University, China</i> Dr. Jielu Yan <i>University of Saint Joseph, Macau, China</i>	
15.45 - 16.00	Break	
16.00 - 16.30 <b>(We leave at 16.30 sharply)</b>	<b>Meeting Point: Universiti LRT Station (KJ19) @16.00</b> <b>(Universiti LRT - Masjid Jamek LRT - KLCC LRT)</b>	
19.00 - 22.00	<b>Meeting Point: KLCC Tower 2 @19.00</b> <b>(Important Document Needed: Passport or IC)</b>	<b>Social Dinner Events (By invitation)</b> <b>Level 43, Seligi Chinese Pavilion</b> Restaurant, Malayan Petroleum Club, KLCC
22.00-23.00	<b>Meeting Point: KLCC Tower 2 @23.00</b> <b>(KLCC LRT - Universiti LRT)</b>	<b>Back to Komune Living</b>

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**9<sup>th</sup> DECEMBER 2023 (SATURDAY)**

**ACSGII & ICCST7**

**Venue: Auditorium,**

**Connexion Event Convention Center (CECC) Bangsar South**

**Level 3A**

**Emcee: Dr. Shameer Bin Hisham (Department of Chemistry, Universiti Malaya)**

8.00 - 8.30	Registration / Breakfast
8.30 - 8.40	<b>Event Inauguration: National Anthem and Prayer</b> Welcome Remarks <b>Professor Dr. Yatimah Binti Alias</b> <i>Deputy Vice-Chancellor (Academic &amp; International), Universiti Malaya</i>
8.40 - 8.45	<b>Dr. Sergio Nanita</b> International Activity Chari - American Chemical Society (IAC - ACS, Zoom)
8.45 - 8.50	<b>Professor Dr. Zulqarnain Mohamed</b> <i>Dean, Faculty of Science, Universiti Malaya</i>
8.50 - 8.55	<b>Professor Dr. Sithi V. Muniandy</b> ACS GII & ICCST7, Quantum Information Science and Technology (QIST) <i>Universiti Malaya</i>
<b>Event Launching / Group Photo Session</b>	
<b>Session: Air Pollution and Environmental Chemistry</b> <b>Chair: Professor Dr. Sithi V. Muniandy (Universiti Malaya)</b> <b>Auditorium</b>	
9:15 - 9:45	<b>Plenary 1: Prof. Emeritus Dato' Dr. Azizan Abu Samah</b> <i>Institute of Ocean and Earth Sciences, Universiti Malaya, Malaysia</i> Topic: Rare Earth Issues and air pollution in the Klang Valley
9.45 - 10.10	<b>Plenary 2: Associate Professor Dr. Somporn Chantara</b> <i>Department of Chemistry, Chiang Mai University, Thailand</i> Topic: Air pollutions in Southeast Asia management, and research challenges
10.10- 10.20	<b>Mrs. Lorraine K.</b> <i>B.A.N.K. Coach and Trainer</i> Topic: Mindful Living: Clearing Mental Clutter for Better Communication
10.20- 10.30	Break
<b>Session: Computational Techniques</b> <b>Chair: Dr. Wai Kit Tang (Universiti Malaya)</b> <b>Auditorium</b>	
10.30 -11.00	<b>Plenary 3: Associate Professor Dr. Chi-Kit SIU</b> <i>Department of Chemistry, City University of Hong Kong, Hong Kong</i> Topic: Computational Modeling of Reaction Mechanisms of Hydrated Ion Clusters toward Atmospheric Gas Molecules
11.00 - 11.30	<b>Plenary 4: Professor Dr. Türkan Haliloğlu</b> <i>Department of Chemical Engineering, Boğaziçi University, Istanbul, Turkey</i> Topic: Deciphering Allosteric Dynamics: Insights from Gaussian Network Analysis
11.30 – 12.00	<b>Plenary 5: Professor Dr. Sun Choi</b> <i>College of Pharmacy and Graduate School of Pharmaceutical Sciences, Ewha Womans University, Seoul-Korea</i> Topic: Molecular Modeling and Artificial Intelligence (AI) assisted Drug Design, and their Applications in Drug Discovery
12.00 - 12.15	<b>Invited Speaker 1: Professor Dr. Yoshi Kawazoe</b> Senior Research Fellow and Professor Emeritus, Tohoku University, Japan Topic: Theory First: From explanation of experiments to a reliable theory to which experimentalists follow (Zoom)
12.15- 14.15	<b>Lunch &amp; Poster Interactive Session</b> <b>Lunch Venue: The Oak Room Bangsar Connexion</b> <b>Poster Venue: Auditorium Foyer</b>

**9<sup>th</sup> DECEMBER 2023 (SATURDAY)****Application Session****Break Room**

	<b>ACSGII</b> <b>Break Room: Reflexion</b> <b>Material Modelling and Simulations</b> <i>Chair: Associate Professor Dr. Rozana Othman</i> <i>(Faculty of Pharmacy, Universiti Malaya)</i>	<b>ICCST7</b> <b>Break Room: Auditorium</b> <b>Pharmaceutical Modelling and Simulations</b> <i>Chair: Dr. Chong Wei Lim</i> <i>(Faculty of Engineering, Universiti Malaya)</i>
14.15 - 14.30	<b>Invited Speaker 2:</b> <b>Assistant Professor Dr. Doan Quang-Van</b> Head of Atmospheric Informatics & Modeling (AIM) Lab, Centre for Computational Sciences, University of Tsukuba, Japan Topic: Future Climate Prediction with High-Performance computer	<b>Invited Speaker 12:</b> <b>Dr. Fransiska Kurniawan</b> School of Pharmacy, Bandung Institute of Technology, Indonesia Topic: Critical Issue in MD Simulation
14.30 - 14.45	<b>Invited Speaker 3:</b> <b>Dr. Marzieh Yaeghoobi</b> Sharoud University of Medicinal Sciences, Iran Topic: Air Quality Modelling	<b>Invited Speaker 13:</b> <b>Professor ChM Dr. Mohd Basyaruddin Abdul Rahman</b> University Putra Malaysia Topic: Biodegradable Calcium-based Metal-organic Frameworks as Nanodelivery of Active Molecules
14.45 - 15.00	<b>Invited Speaker 4:</b> <b>Professor Dr. Thomas Lei</b> University of Saint Joseph, Macao, China Topic: Application of ANN, XGBoost, and Other ML Methods to Forecast Air Quality in Macau	<b>Invited Speaker 14:</b> <b>Professor Dr. rer. nat. apt. Sophi Damayanti</b> School of Pharmacy, Bandung Institute of Technology, Indonesia Topic: The Role of Computational Chemistry in Developing Molecular Imprinted Polymer for Separation Method
15.00 - 15.15	<b>Invited Speaker 5:</b> <b>Professor Dr. Lee-Wei Yang</b> National Tsing Hua University, Taiwan Topic: Integration of on-target and systemic chemical fragments of old drugs in CADD to save the environment and lives	<b>Invited Speaker 15:</b> <b>Associate Professor Dr. Hisashi Okumura</b> Institute for Molecular Science, Japan Topic: Disease-related Protein Studied by Molecular Dynamics Simulations
15.15 - 15.30	<b>Invited Speaker 6:</b> <b>Professor Dr. Juan Joon Ching</b> NANOCAT, Universiti Malaya, Malaysia Topic: Removing Harmful VOC with Light Energy	<b>Invited Speaker 16:</b> <b>Associate Professor Dr. Bimo Ario Tejo Universiti Putra Malaysia</b> Topic: Challenges and Opportunities in Designing Drugs for Tuberculosis
15.30 - 15.45	<b>Invited Speaker 7:</b> <b>Professor Dr. Darwin Barayang Putungan,</b> Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, Title: Hydrogen Evolution Reaction on Bulk and 2D Materials: The Role of Surface Features and Structural Phase (Zoom)	<b>Invited Speaker 17:</b> <b>Dr. Bilal Shaker</b> Global AI Drug Discovery Center, College of Pharmacy and Graduate School of Pharmaceutical Sciences, Ewha Womans University, Korea Topic: Identification of Positive Allosteric Modulators (PAMs) for the A1 Adenosine Receptor (A1AR) Using Pharmacophore Modeling and Molecular Dynamics Simulations: A Comprehensive Drug Discovery Approach
15.45 - 16.00	<b>Break</b>	

	<b>ACSGII</b> <b>Break Room: Reflexion</b>	<b>ICCST7</b> <b>Break Room: Auditorium</b>
16.00 - 16.15	<p><b>Chair: Dr. Vijayan Manickam Achari, Institute of Biological Science (ISB), Universiti Malaya</b></p> <p><b>Invited Speaker :8</b> <b>Associate Professor Dr. Piyarat Nimmanpipug</b> Chiang Mai University, Chiang Mai, Thailand Topic: Supramolecular Functional Materials Simulations for Sustainability</p>	<p><b>Chair: Professor Dr. rer. nat. apt. Sophi Damayanti I, School of Pharmacy, Bandung Institute of Technology, Indonesia</b></p> <p><b>Invited Speaker 18:</b> <b>Assistant Professor Dr. Satoru Itoh</b> Institute for Molecular Science, Japan Topic: Generalized-ensemble Algorithms for Protein Oligomerization Processes</p>
16.15 - 16.30	<p><b>Invited Speaker 9:</b> <b>Associate Professor Dr. Yeoh Keat Hoe</b> Jeffrey Sachs Centre on Sustainable Development, Sunway University Topic: Theoretical Screening of Single Transition Metal Atom Substitutional Doped on Monolayer Nb<sub>2</sub>S<sub>2</sub>C for Oxygen Reduction Reaction</p>	<p><b>Invited Speaker 19:</b> <b>Associate Professor Dr. Phornphimon Maitarad</b> Shanghai University, China Topic: Comparative Study of Machine-Learning-Based QSAR Modeling of Anti-Inflammatory Compounds from Durian Extraction</p>
16.30 - 16.45	<p><b>Invited Speaker 10:</b> <b>Associate Professor Dr. Low Kah Hin</b> Universiti Malaya, Malaysia Topic: Reinventing Waste Optical Discs Into Polycarbonate-based Adsorbents: Response Surface Methodology in Adsorption Study</p>	<p><b>Invited Speaker 20:</b> <b>Professor Dr. Supat Jiranusornkul</b> Chiang Mai University, Chiang Mai, Thailand Topic: Multitarget Virtual Screening For Potential Herbal Substances Against Osteoporosis</p>
16.45 - 17.00	<p><b>Invited Speaker 11:</b> <b>Associate Professor Dr. Sarah Harris (Zoom)</b> University of Leeds, United Kingdom Topic: Coarse Grained FFEA</p>	<p><b>Invited Speaker 21:</b> <b>Dr. Jielu Yan</b> University of Saint Joseph, Macau, China Topic: MBC-Attention: A Deep Learning Method For Predicting the Minimum Inhibitory Concentration of antimicrobial peptides against Escherichia coli using Multi-Branch-CNN and Attention</p>
17.00 – 18.00	<p><b>Chair: Professor Dr. Sithi V. Muniandy and Associate Professor Dr. Vannajan S. Lee (Universiti Malaya)</b></p> <p><b>Networking Session (Invited Guest)</b> <b>Venue: Reflexion</b></p> <ul style="list-style-type: none"> <li>• <b>Asian Federal Medicinal Chemistry (AFMC)</b></li> <li>• <b>Blockchain in Computer Aided Molecular Design CAMD</b></li> </ul>	
18.00 - 21.00	<p><b>Conference Dinner (The Oak Room Bangsar Connexion)</b></p>	

<b>10<sup>th</sup> DECEMBER 2023 (SUNDAY)</b> <b>HPC and New Trends Session</b> <b>Auditorium</b>	
8:30 - 9:00	Breakfast
9:00 - 9:15	<b>Chair: Dr. Siti Jariani Mohd. Jani</b> <b>Department of Chemistry, Universiti Malaya</b> <b>Invited Speaker 22: Roslan Abdul Wahab</b> <i>Cofounder, SynergyLabs MY ICP.Hub</i> Topic: Application of Blockchain to Air Pollution Data Gathering
9:15 - 9:30	<b>Invited Speaker 23: Associate Professor Dr. Liew Chee Sun</b> <i>Head of Data Intensive Computer Centre (DICC), Malaysia</i> Topic: Facilitating Scientific Discovery using Advanced Computing
9:30 - 9:45	<b>Invited Speaker 24: Dr. Nurzatil Sharleeza Mat Jalaluddin</b> <i>Ex-officio Malaysia Open Science Alliance member</i> Topic: Open Science for Impactful Research
9:45 - 10.00	<b>Invited Speaker 25: Professor Dr. Arry Yanuar</b> <i>Faculty of Pharmacy, Universitas Indonesia, Indonesia</i> Topic: Computational Approach in Green Chemistry
10.00 - 10.30	<b>Plenary 6: Professor Dr. Andriyan Bayu Suksmono</b> <i>School of Electrical Engineering and Informatics, Bandung Institute of Technology, Indonesia</i> Topic: An Introduction to the 2nd Quantum Revolution and Quantum Computing
10.30 - 10.45	<b>Invited Speaker 26: Dr. Nils Herrmann</b> <i>Quantum Brilliance</i> Topic: Quantum Chemistry on NV-center based qubits in diamond (Zoom)
<b>10.45 – 11.00</b>	<b>Break</b>
11.00 – 11.15	<b>Chair: Dr. Choon Han Heh, Faculty of Pharmacy, Universiti Malaya</b> <b>Invited Speaker 27: Professor Dr. Moritz Mueller</b> <i>Swinburne University, Australia (Malaysia campus)</i> Topic: The Power of Data Cubes in Earth Observation
11.15 – 11.30	<b>Invited Speaker 28: Associate Professor Dr. Davood Tofighi</b> <i>University of New Mexico, USA</i> Topic: Impacts of Environmental Pollution on Public Health: A Critical Review (Zoom)
11.30 – 11.45	<b>Invited Speaker 29: Associate Professor Dr. Jane Gew Lai Ti</b> <i>Sunway University, Malaysia</i> Topic: Towards Zero Single-Use Plastics: The Role of Chemistry Knowledge
11.45 -12.00	<b>Invited Speaker 30: Professor Dr. U Deva Priyakumar</b> <i>Centre for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, CCNSB, IIT Campus, Gachibowli, Hyderabad, India</i> Topic: Impact of AI/ML in Healthcare: Screening, Diagnosis and Prognosis
12.00 - 12.15	<b>Invited Speaker 31: Associate Professor Dr. Thanyada Rongrutmongkul</b> <i>Chulalongkorn University, Thailand</i> Topic: Designing SARS-CoV-2 Main Protease Inhibitors with Enhanced Experimental Inhibitory Efficiency Using Machine Learning-based QSAR and LB-PaCS-MD
12.15 - 12.30	<b>Invited Speaker 32: Dr. Yasmin Binti Shamsudin</b> <i>Uppsala University, Sweden</i> Topic: Going Green- Computer-Aided Engineering of Green Fluorescent Proteins
12.15 -12.45	<b>Closing Ceremony</b> <b>Chair: Associate Professor Dr. Woi Pei Meng, Universiti Malaya</b> <b>Kureka MakerSpace@UM AI awards</b> <b>ACS Social Media Master Award</b> <b>ACS Poster awards winner</b>
12.45-14.30	Lunch (The Oak Room Bangsar Connexion)
14.30-15.30	<b>ACS UM Student Get Together    Venue: Reflexion</b>
15.30-22.00	Excursion: Firefly Sanctuary <b>Meeting Point: Komune Living @15.30</b> <b>(Prebooking at Reception: The bus leaves at 16.00 sharply)</b>