COMPUTATIONAL AND EXPERIMENTAL CHEMISTRY: DEVELOPMENT AND APPLICATION

VIRTUAL PRESENTATIONS

26 AUGUST 2021

University of Johannesburg
Chemical Sciences
Faculty of Sciences
Johannesburg
South Africa

Tohoku University
Frontier Research Institute of
Interdisciplinary Sciences
Sendai
Japan

Foreword

Computational chemistry is a branch of chemistry that uses computer simulation to assist in solving complex chemical problems. It exploits methods of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures, the interactions, and the properties of molecules. This support system of Experimental and computational chemistry makes it possible to obtain high quality results theoretically and experimentally. The presentations are a part of a continuous collaboration between University of Johannesburg (South Africa) and Tohoku University (Japan). The collaboration aims to solidify knowledge exchange in the broader scope of forging long-lasting nexus between the two universities and countries through student exchange, co-supervision, co-publication, and bilateral agreements within the context of energy research.

Programme (Registration: https://tinyurl.com/UJRI-IOV) Zoom ID: 89509786494 PW: 668143

TIME	TITTLE	SPEAKER	UNIVERSITY
Session 1: Chair: Dr Phumlani Msomi (University of Johannesburg)			
8:00 – 8:05	Welcome address	Prof James Ramontja (Department HOD)	University of Johannesburg
8:05 – 8:20	Molecular simulation of ionomer self-assembly for fuel cell application	Dr Takuya Mabuchi	Tohoku University
8:20 – 8:35	Synthesis and characterization of an ionomer to study its effects on direct alcohol fuel cell catalysts	Ms Thandiwe Maumau	University of Johannesburg
8:35 – 8:50	Role of geochemical modeling in the water quality monitoring	Dr Martin Magu	Multimedia University of Kenya

8:50- 9:05	Identification of small organic molecules as potential inhibitors for COVID-19 main protease enzyme.	Dr Ephraim Marondedze	University of Johannesburg

TIME	TITTLE	SPEAKER	UNIVERSITY
Session 2: Chair: Dr Zikhona Tywabi-Ngeva (Nelson Mandela University)			
9:10 – 9:25	Experimental studies of transportation phenomena in catalyst inks and catalyst layers	Dr Takahiro Suzuki	Osaka University
9:25 – 9:40	Electrocatalytic activity of alumina-silicates supported electrocatalysts for oxygen reduction reaction in alkaline media	Ms Teboho Mashola	University of Johannesburg
9:40 – 9:55	Application of metal oxide carbon nano-particles cellulose acetate-based gas sensors for the detection of tuberculosis biomarkers	Mr Lesego Malepe	University Johannesburg
9:55 – 10:10	Systematic tuning of fluorescence Stokes shift of Re(I) complexes of 12H-indazolo[5,6-f][1,10] phenanthroline: a TDDFT study of substituent and solvent effects	Dr Olawale Olasunkanmi	University of Johannesburg

TIME	TITTLE	SPEAKER	UNIVERSITY
Session 3: Chair: Dr Takuya Mabuchi (Tohoku University)			
10:15 – 10:30	Non-precious metal molecular catalyst on carbon for oxygen reduction reaction	Dr Hiroya Abe	Tohoku University
10:30 – 10:45	Studies on the catalytic properties of metal electro-catalysts supported on carbon-based nanomaterials towards alcohol electro oxidation in alkaline medium	Ms Memory Zikhali	University of Johannesburg
10:45 – 11:00	Synthesis and characterization of modified transition metal dichalcogenides towards photodegradation of personal care products in water	Mr Justice Mphahlele	University Johannesburg
Organizers Dr Phumlani Msomi, University of Johannesburg, RSA Dr Takuya Mabuchi, Tohoku University, Japan			