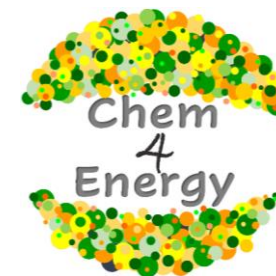


Chem4Energy Annual Conference
Materials and Processes for a Sustainable Energy Future
Wednesday 20 – Sunday 24 March 2024



Conference Programme (may be subject to amendment)

Wednesday 20 March 2024

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| 14:30 – 15:45 | <i>Registration & Refreshments</i> | |
| 15:45 – 16:00 | Welcome and Opening | Prof Nora de Leeuw University of Leeds, UK; Utrecht University, The Netherlands |
| 16:00 – 16:45 | Keynote High Performance Computing Developments in South Africa | Dr Happy Sithole Center Manager: National Integrated Cyber-Infrastructure at CSIR (NICIS), South Africa |
| 16:45 – 17:10 | DFT study of hydrogen adsorption on fcc ruthenium surfaces | <u>Marietjie Ungerer</u> , Cardiff University, UK; Nora de Leeuw, University of Leeds, UK; |
| 17:10 – 17:35 | The effect of small amount of Nb on FeCo soft magnetic alloy: A computational study | <u>Ramogohlo Diale</u> , Joseph Moema and Maje Phasha, MINTEK, South Africa; Phuti Ngoepe and Hasani Chauke, University of Limpopo, South Africa |
| 17:35 – 18:00 | Carbon as a chemical or an energy source? A philosophical view | <u>Wynand Serfontein</u> , North-West University, South Africa |
| 18:00 | <i>Close of session</i> | |
| 19:00 | Dinner | |

Thursday 21 March 2024

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| 08:50 – 09:00 | <i>Chair's comments</i> | <i>Professor Scott Woodley</i> |
| 09:00 – 09:45 | Keynote Atomic scale simulation and nuclear fuel performance | Professor Robin Grimes Imperial College London, UK |
| 09:45 – 10:10 | Optoelectronic simulation properties of modified tin oxide nanostructure for solar cell application | <u>Gugu Kubheka</u> and Mpho Lekgoathi, South African Nuclear Energy Corporation (Necsa), South Africa |
| 10:10 – 10:35 | Theoretical investigations on point defects in BaSnO ₃ using a Mott-Littleton method | <u>Zhe Xu</u> , Alexey Sokols and Scott Woodley, University College London, UK |
| 10:35 – 11:00 | Heteroepitaxial α -Al ₂ O ₃ /LiMn ₂ O ₄ interfaces: structures, electronic and delithiation thermodynamics properties | <u>Brian Ramogayana</u> , Khomotso P Maenetja and Phuti E Ngoepe, University of Limpopo, South Africa; David Santos-Carballal and Nora H. De Leeuw, University of Leeds, UK |
| 11:00 – 11:30 | <i>Refreshment break</i> | |
| 11:30 – 11:55 | Formation and catalytic activity of 1D gold oxide chains from density functional theory | <u>Lyudmila Moskaleva</u> and Lenard Carroll, University of the Free State, South Africa |
| 11:55 – 12:20 | Saccharin as a green catalytic component for the CO ₂ fixation into propylene carbonate: A comprehensive DFT study | Teshome A Lelisho, Hawassa University, Ethiopia; Jean Du Toit and <u>Cornie Van Sittert</u> , North-West University, South Africa |
| 12:20 – 12:45 | Mechanism of ammonia synthesis on Ni ₂ Mo ₃ N(111) | <u>Michael Higham</u> and Richard Catlow, University College London, UK; Angela Daisley and Justin Hargreaves, University of Glasgow, UK |
| 12:45 – 14:00 | <i>Lunch</i> | |
| 14:00 – 14:10 | <i>Chair's comments</i> | <i>Professor Phuti Ngoepe</i> |
| 14:10 – 14:55 | Keynote Sustainable batteries and electrocatalytic processes | Professor Magda Titerici Imperial College London, UK |
| 14:55 – 15:20 | Synthesis and characterisation of multi-walled carbon nanotubes for lithium-ion batteries | <u>Nqobile Mhlanga</u> , Mpfunzeni Raphulu and Thembisile Khumalo, MINTEK, South Africa; Vusumuzi Sibanda, University of the Witwatersrand, South Africa |
| 15:20 – 15:45 | The photon-electrical conversion efficiency of dye-sensitive solar cells fabricated using silver-nanoparticle/titania photocathode | <u>Likius Shipwiisho Daniel</u> , Ateeq Rahman, Kalegay Mbela, Veikko Uahengo, Loini Kalipi and Rocha Tephken Kaffer, University of Namibia, Namibia |
| 15:45 – 16:15 | <i>Refreshment Break</i> | |
| 16:15 – 16:40 | Titanium dioxide nanotubes synthesis and application as anode materials for potassium-ion batteries | <u>Thembisile Khumalo</u> , Athule Ngqalakwezi, Nqobile Mhlanga, Gary Patrick and Mpfunzeni Raphulu, MINTEK, South Africa |
| 16:40 – 17:05 | Chain propagation and termination in the low-temperature combustion of n-alkanes | <u>Kgalaletso Otukile</u> , Cameron Matthews and Lyudmila Moskaleva, University of the Free State, South Africa; Saurabh Kandpal, Sabyasachi Chakraborty and Raghunathan Ramakrishnan, Tata Institute of Fundamental Research, India |
| 17:05 – 17:30 | Synthesis, spectroscopic and electrochemical behaviour of a series of ferrocene-bearing dodecylphthalocyanines | <u>Glendin Swart</u> , Eleanor Fourie-Müller, Jannie C. Swarts |
| 17:30 – 19:00 | Poster Session | |
| 19:30 | <i>Dinner</i> | |

Friday 22 March 2024

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| 08:50 – 09:00 | <i>Chair's comments</i> | <i>Professor Cornie van Sittert</i> |
| 09:00 – 09:45 | Keynote Utilisation of ionic liquids and catalysis for net zero applications | Professor Chris Hardacre University of Manchester, UK |
| 09:45 – 10:10 | Performance of Pt ternary alloys as ORR electrocatalysts | Thelma Ngwenya and <u>Zicabangele Mseleku</u> , MINTEK, South Africa |
| 10:10 – 13:35 | Investigating high entropy alloys for hydrogen storage | <u>Jacuguline Tau</u> , Rosinah Modiba, Ntombizodwa Mathe, Nana Arthur and Sisa Pityana, CSIR, South Africa; Charles W Siyasiya, University of Pretoria, South Africa |
| 10:35 – 11:00 | Hydrogen evolution reaction on polyaniline modified with metal organic framework and molybdenum disulphide in acidic medium | Kabelo Edmond Ramohlola, Miranda Ndipingwi and Emmanuel Iwuoha, University of Western Cape, South Africa; Kwena Desmond Modibane, University of Limpopo, South Africa |
| 11:00 – 11:30 | <i>Refreshment break</i> | |
| 11:30 – 11:55 | Metal-exchanged ZIF-8 and ZIF-67 nanoparticles with enhanced catalytic activity | <u>Ernst Langner</u> , Lehlohonolo Mphuthi and Elizabeth Erasmus, University of the Free State, South Africa; Mametsi Maseme, Walter Sisulu University, South Africa |
| 11:55 – 12:20 | Sustainability in fuel and petrochemical production: exploring novel ZSM-5 catalysts for enhanced clean energy production | <u>Smarte Anekwe</u> and Yusuf Isa, University of the Witwatersrand, South Africa; Bilainu Oboirien, University of Johannesburg, South Africa |
| 12:20 – 12:45 | Improved ORR activity of Pt on N-doped Ketjenblack for PEM fuel cells | Thelma Ngwenya and <u>Katlego Tshehla</u> , MINTEK, South Africa |
| 12:45 – 14:00 | <i>Lunch</i> | |
| 14:00 – 14:10 | <i>Chair's comments</i> | <i>Professor Lyudmila Moskaleva</i> |
| 14:10 – 14:55 | Keynote Studies of metal-ion batteries active materials using multiscale scale simulations | Professor Phuti Ngoepe Director: Materials Modelling Centre, University of Limpopo, South Africa |
| 14:55 – 15:20 | Towards a rational design of novel green catalysis: a computational perspective from the UK Catalysis Hub | <u>Matthew Quesne</u> and C. Richard Catlow, Cardiff University, UK |
| 15:20 – 15:45 | Modelling TiO ₂ -supported subnanometer-sized metal clusters confined in zeolite cavities | Sabelo Cele, <u>Cameron Matthews</u> and Lyudmila Moshaleva, University of the Free State, South Africa |
| 15:45 | <i>Close of Session</i> | |
| 16:30 | <i>Game Drive</i> | |
| 19:00 | <i>Braai</i> | <i>Boma</i> |

Saturday 23 March 2024

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| 08:50 – 09:00 | <i>Chair's comments</i> | <i>Professor Chris Hardacre</i> |
| 09:00 – 09:45 | Keynote Catalysts for CO removal from hydrogen | Professor Patricia Kooyman SARCHI Chair in Nanomaterials for Catalysis, University of Cape Town, South Africa |
| 09:45 – 10:10 | Application of platinum-alloy nanostructures to enhance ORR activity in PEMFCs | <u>Siphelo Ngqoloda</u> and Thelma Ngwenya, MINTEK, South Africa |
| 10:10 – 10:35 | Evaluation of Mo-promoted Ni/AC catalysts in CO ₂ methanation: effect of different synthesis method | <u>Stephen Akpasi</u> and Thembisile Mahlangu, Durban University of Technology; South Africa; Yusuf Isa, University of Witwatersrang, South Africa; Sammy Kiambi, Vaal University of Technology, South Africa |
| 10:35 – 11:00 | MnxNi _{1-x} oxide electrocatalysts for the oxygen evolution reaction in alkaline media | <u>Fariya Moosa</u> , Tarisai Velepini and Anzel Falch, University of the Witwatersrand, South Africa |
| 11:00 – 11:30 | <i>Refreshment break</i> | |
| 11:30 – 11:55 | Photocatalytic studies of ruthenium-based dyes for solar cells: a precursor for GH ₂ production from H ₂ O | <u>Veikko Uahengo</u> , Johannes Naimhwaka, Paulina Endjala, Likius Daniel and Ateeq Rahman, University of Namibia, Namibia |
| 11:55 – 12:20 | Water-mediated synthesis of niobium doped BiOI for photocatalytic degradation of methyl orange | <u>Sive Nosenga</u> and Phindile Khoza, University of Kwazulu-Natal, South Africa |
| 12:20 – 12:45 | Trialkylphosphine-mediated transformation of nickel sulphides to phosphides for water splitting | <u>Gwaza Eric Ayom</u> and Neerish Revaprasadu, University of Zululand, South Africa |
| 12:45 – 14:00 | <i>Lunch</i> | |
| 14:00 – 14:10 | <i>Chair's comments</i> | <i>Dr Happy Sithole</i> |
| 14:10 – 14:55 | Keynote Computational modelling of materials and processes for a sustainable energy future | Professor Richard Catlow University College London, UK |
| 14:55 – 15:20 | Dimerization and confinement of Cu ₅ clusters on pristine and defected graphene | <u>Lenard Carroll</u> and María Pilar de Lara-Castells, Consejo Superior de Investigaciones Científicas (CSIC), Spain; Lyudmila Moskaleva, University of the Free State, South Africa |
| 15:20 – 15:45 | DFT study of monoclinic FeNbO ₄ : bulk properties and water dissociation reaction | <u>Xingyu Wang</u> , David Santos-Carballal, Nora de Leeuw, University of Leeds, UK |
| 15:45 – 16:15 | <i>Refreshment break</i> | |
| 16:15 – 16:40 | Development of an electrocatalyst to produce green hydrogen from water electrolysis: DFT study | <u>Sabelo Jeza</u> , Amir Hossein Mohammadi, David Lokhat and Cornelia Gertina Catharina Elizabeth Van Sittert, University of KwaZulu-Natal, South Africa |
| 16:40 – 17:05 | Hydrogen adsorption on Pt doped titanium clusters TiN-1Pt (N = 2-16) | <u>Tshegofatso Michael Phaahla</u> , Phuti Esrom Ngoepe and Hasani Richard Chauke, University of Limpopo, South Africa |
| 17:05 – 17:30 | Water adsorption on (010) and (101) CuWO ₄ surfaces | <u>Xuan Chu</u> , David Santos-Carballal, Nora H de Leeuw, University of Leeds, UK |
| 17:30 | Closing remarks | Prof Cornie van Sittert, North-West University, South Africa |

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| 17:45 | Close of conference | |
| 19:30 | Conference Dinner & Interactive Drumming | Lobola Restaurant |

Sunday 24 March 2024

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| 07:00 | Early Transport departs (only for delegates that need to be at Lanseria International Airport by 08.00 or O.R Tambo International Airport by 09.00) |
| Before 10:00 | Check out |
| 11:00 | Transport departs to Lanseria International Airport and O.R Tambo International Airport |