

Computation for Applied Catalysis Workshop

Monday 10th – Wednesday 12th March 2025

University of Leeds, UK

| Monday 10 th March: Bragg SR GR.18 | |
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| 12.10-13.00 | Registration and Lunch: Mechanical Engineering Foyer |
| 13.00-13.05 | Welcome and Introduction: Prof. Richard Catlow , University College London and Cardiff University |
| 13.05 -13.55 | <u>Plenary talk</u> Prof. Karsten Reuter , Fritz-Haber-Institut der Max-Planck-Gesellschaft <i>Machine learning accelerated materials discovery for energy conversion and storage</i> |
| | Session 1 Chair: Prof. David Willock , Cardiff University |
| 13.55-14.15 | Matt Robinson , Cardiff University <i>Tuning zeolite catalysts using Organic Additives</i> |
| 14.15-14.35 | Dr. Jingcheng Guan , University College London <i>Methanol Loading Induced Protonation as Activation for MTH Process in Zeolite ZSM-5</i> |
| 14.35-14.55 | Prof. Feng-Yuan Zhang , University of Tennessee <i>In-operando and comprehensive characterizations of electrocatalysts for electrolysis technology</i> |
| 14.55-15.30 | Refreshments: Mechanical Engineering Foyer |
| 15.30-16.20 | <u>Plenary talk</u> Prof. Mercedes Boronat , Instituto de Tecnología Química <i>New developments in the molecular modelling of zeolites for heterogeneous catalysis</i> |
| 16.20-16.40 | Akash Hiregange , Cardiff University <i>Computational insights into stability and phase transition of cobalt oxide nanoparticles for Fischer-Tropsch catalysts</i> |
| 16.40-17.00 | Thomas Hill , Cardiff University <i>Metal oxides and DFT: a CeO₂ and TiO₂ study</i> |
| 17.00-19.00 | Poster session and refreshments: Mechanical Engineering Foyer |

| Tuesday 11th March: Civil Eng LTB 3.25 | |
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| | Session 2 Chair: Dr. Umberto Terranova , University of Buckingham |
| 09.00-09.50 | <u>Plenary talk</u> Prof. Paul Donaldson , University of Liverpool, Central Laser Facility <i>Recent progress towards making the connection between ultrafast spectroscopy and computation for catalysis</i> |
| 09.50-10.10 | Dr. Marietjie J. Ungerer , University of Leeds <i>Ruthenium fcc surfaces and nanoparticles for hydrogen and nitrogen production</i> |
| 10.10-10.50 | Refreshments: Mechanical Engineering Foyer |
| 10.50-11.10 | Dr. Xue Yong , University of Liverpool <i>Bi-layer single atom catalysts boosted nitrate-to-ammonia electroreduction with high activity and selectivity</i> |
| 11.10-11.30 | Dr. Jamal Abdul Nasir , University College London <i>Selective catalytic reduction of nitrogen oxides with ammonia over Cu-CHA and Fe-BEA zeolite</i> |
| 11.30-11.50 | Dr. Alexander D. James , University of Leeds <i>Pollutants interaction with the major surfaces of hematite α-Fe₂O₃</i> |
| 11.50-12.10 | Dr. Michael Higham , University College London <i>Amide-rich NaH as a highly active catalyst for ammonia synthesis</i> |
| 12.10-13.10 | Lunch: Mechanical Engineering Foyer |
| | Session 3 Chair: Dr. Alexey Sokol , University College London |
| 13.10 -14.00 | <u>Plenary talk</u> Dr. Elisa Borfecchia , University of Turin <i>Shedding light on Cu-CHA deNO_x catalysts by X-ray spectroscopy</i> |
| 14.00-14.20 | Dr. Kaifeng Niu , University of Cambridge <i>CO₂ hydrogenation with high selectivity by single bi atoms on MXenes enabled by a concerted mechanism</i> |
| 14.20-14.40 | Shijia Sun , University College London <i>Comparative analysis of the mechanism and selectivity of CO₂ hydrogenation on pure and Fe-promoted Rh (111) surfaces</i> |
| 14.40-15.00 | Inioluwa C. Popoola , University of Cambridge <i>Cooperative CO₂ capture via oxalate formation on metal-decorated graphene</i> |
| 15.00-15.20 | Dr. David Santos-Carballal , University of Leeds <i>Single-atom catalysis and electrostatic fields for CO₂ dissociation</i> |
| 15.20-16.00 | Refreshments: Mechanical Engineering Foyer |
| 16.00-16.50 | Dr. Matthew Quesne , University of Leeds <i>Computation for a green future: exploring the length vs time scale</i> |
| 16.50-17.10 | Dr. Fabian Berger , University of Cambridge <i>Two are better than one: exploring single and dual active sites in the novel material class of highly dispersed ternary alloys</i> |
| 17.10-17.30 | Yuxiang Cai , University of Liverpool <i>Improving molecule-metal surface reaction networks using the meta-generalized gradient approximation: CO₂ hydrogenation</i> |
| 17.30-18.20 | <u>Plenary talk</u> Prof. Nora de Leeuw , University of Leeds <i>Density functional theory study of the catalysed tautomerization of phenol by Zeolite MFI</i> |
| 18.30-22.30 | Pre-dinner refreshments (18.30-19.00) Conference dinner (19.00-22.30) University House |

| Wednesday 12th March: Bragg SR GR.18 | |
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| | Session 4 Chair: Dr. Matthew Quesne , University of Leeds |
| 09.00-09.50 | <u>Plenary talk</u> Prof. Gianfranco Pacchioni , University of Milano-Bicocca <i>Modelling single-atom catalysts</i> |
| 09.50-10.10 | Eimear McCarthy , Cardiff University <i>CO₂ hydrogenation at the Pd/ZnO interface</i> |
| 10.10-10.50 | Refreshments: Mechanical Engineering Foyer |
| 10.50-11.10 | Dr. Natalia Martsinovich , The University of Sheffield <i>Mechanisms of photocatalytic conversion of methane to ethane on TiO₂ with Pd-based co-catalysts</i> |
| 11.10-11.30 | Matthew Wigglesworth , The University of Sheffield <i>A theoretical perspective on hydrogen evolution through photoreforming of methanol on metal-loaded anatase (101)</i> |
| 11.30-12:20 | <u>Plenary talk</u> Prof. Emiel Hensen , Eindhoven University of Technology TBD |
| 12.20-12.30 | Prof. Colin Fishwick , University of Leeds Closing remarks |
| 12:30 | Lunch and Close: Mechanical Engineering Foyer |