Computation for Applied Catalysis Workshop

Monday 10th – Wednesday 12th March 2025

University of Leeds, UK

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

Tuesday 11th March: Civil Eng LTB 3.25	
	Session 2 Chair: **Dr. Umberto Terranova**, University of Buckingham
09.00-09.50	Plenary talk **Prof. Paul Donaldson**, University of Liverpool, Central Laser Facility *Recent progress towards making the connection between ultrafast spectroscopy and computation for catalysis*
09.50-10.10	**Dr. Marietjie J. Ungerer**, University of Leeds *Ruthenium fcc surfaces and nanoparticles for hydrogen and nitrogen production*
10.10-10.50	**Refreshments:** Electrical Engineering Foyer
10.50-11.10	**Dr. Xue Yong**, University of Liverpool *Bi-layer single atom catalysts boosted nitrate-to-ammonia electroreduction with high activity and selectivity*
11.10-11.30	**Dr. Jamal Abdul Nasir**, University College London *Selective catalytic reduction of nitrogen oxides with ammonia over Cu-CHA and Fe-BEA zeolite*
11.30-11:50	**Dr. Alexander D. James**, University of Leeds *Pollutants interaction with the major surfaces of hematite α-Fe_2O_3*
11.50-12.10	**Dr. Michael Higham**, University College London *Amide-rich NaH as a highly active catalyst for ammonia synthesis*
12.10-13.10	**Lunch:** Electrical Engineering Foyer
	Session 3 Chair: **Dr. Alexey Sokol**, University College London
13.10 -14.00	Plenary talk **Dr. Elisa Borfecchia**, University of Turin *Shedding light on Cu-CHA deNO_x catalysts by X-ray spectroscopy*
14.00-14.20	**Dr. Kaifeng Niu**, University of Cambridge *CO_2 hydrogenation with high selectivity by single bi atoms on MXenes enabled by a concerted mechanism*
14.20-14.40	**Shijia Sun**, University College London *Comparative analysis of the mechanism and selectivity of CO_2 hydrogenation on pure and Fe-promoted Rh (111) surfaces*
14.40-15.00	**Inioluwa C. Popoola**, University of Cambridge *Cooperative CO_2 capture via oxalate formation on metal-decorated graphene*
15.00-15.20	**Dr. David Santos-Carballal**, University of Leeds *Single-atom catalysis and electrostatic fields for CO_2 dissociation*
15.20-16.00	**Refreshments:** Electrical Engineering Foyer
16.00-16.50	**Dr. Matthew Quesne**, University of Leeds *Computation for a green future: exploring the length vs time scale*
16.50-17.10	**Dr. Fabian Berger**, University of Cambridge *Two are better than one: exploring single and dual active sites in the novel material class of highly dispersed ternary alloys*
17.10-17.30	**Yuxiang Cai**, University of Liverpool *Improving molecule-metal surface reaction networks using the meta-generalized gradient approximation: CO_2 hydrogenation*
17.30-18.20	Plenary talk **Prof. Nora de Leeuw**, University of Leeds *Density functional theory study of the catalysed tautomerization of phenol by Zeolite MFI*
18.30-22.30	**Pre-dinner refreshments** (18.30-19.00) **Workshop dinner** (19.00-22.30) **University House**

Wednesday 12th March: Electrical Engineering Rhodes Lecture Theatre (G.55)	
	Session 4 Chair: **Prof. David Willock**, Cardiff University
09.00-09.50	Pleneray talk **Prof. Gianfranco Pacchioni**, University of Milano-Bicocca *Modelling single-atom catalysts*
09.50-10.10	**Zhongwei Lu**, Cardiff University *Subgroup discovery points to merits of ideal Cu-based diluted alloy for CO_2 hydrogenation*
10.10-10.50	**Refreshments:** Electrical Engineering Foyer
10.50-11.10	**Dr. Natalia Martsinovich**, The University of Sheffield *Mechanisms of photocatalytic conversion of methane to ethane on TiO2 with Pd-based co-catalysts*
11.10-11.30	**Matthew Wigglesworth**, The University of Sheffield *A theoretical perspective on hydrogen evolution through photoreforming of methanol on metal-loaded anatase (101)*
11.30-12:20	Plenary talk **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:** Electrical Engineering Foyer