Computation for Applied Catalysis Workshop

Monday 10th – Wednesday 12th March 2025

University of Leeds, UK

Monday 10 th 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

Session 2 Chair: Dr. Umberto Terranova, University of Buckingham Plenary talk Prof. Paul Donaldson, University of Liverpool, Central Laser Facility Recent progress towards making the connection between ultrafast spectroscopy and computation for catalysis 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 Dr. Xue Yong, University of Liverpool Bi-layer single atom catalysts boosted nitrate-to-ammonia electroreduction with high activity and selectivity Dr. Jamal Abdul Nasir, University College London Selective catalytic reduction of nitrogen oxides with ammonia over Cu-CHA and Fe- BEA zeolite Dr. Alexander D. James, University of Leeds Pollutants interaction with the major surfaces of hematite a-Fe ₂ O ₃ Dr. Michael Higham, University College London Amide-rich NaH as a highly active catalyst for ammonia synthesis Lunch: Electrical Engineering Foyer Session 3 Chair: Dr. Alexey Sokol, University College London Plenary talk Dr. Elisa Borfecchia, University of Turin Shedding light on Cu-CHA deNO, catalysts by X-ray spectroscopy Dr. Kaifeng Niu, University of Cambridge CO ₂ hydrogenation with high selectivity by single bi atoms on MXenes enabled by a concerted mechanism Shijia Sun, University College London Comparative analysis of the mechanism and selectivity of CO ₂ hydrogenation on pure and Fe-promoted Rh (111) surfaces Inicluwa C. Poppola, University of Cambridge Cooperative CO ₂ capture via oxalate formation on metal-decorated graphene Dr. David Santos-Carballat, University of Leeds Single-atom catalysis and electrostatic fields for CO ₂ dissociation Refreshments: Electrical Engineering Foyer Two are better than one: exploring single and dual active sites in the novel material class of highly dispersed ternary alloys Yuxiang Cal, University of Liverpool Improving molecule-metal surface reaction networks using the meta-generalized gradient approximation: CO ₂ hydrogenation Plenar	Tuesday 11th March: Civil Eng LTB 3.25		
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, I I I I I I I I I I I I I I I I	17.30-18.20	Prof. Nora de Leeuw, University of Leeds	
Density functional theory study of the catalysed tautomerization of phenol by Zeolite MFI	33 -3.20	·	
Pre-dinner refreshments (18.30-19.00)			
18.30-22.30 Workshop dinner (19.00-22.30)	18.30-22.30	·	
·		University House	

Wednesday 12th March: Electrical Engineering Rhodes Lecture Theatre (G.55)		
	Session 4 Chair: Prof. David Willock , Cardiff University	
09.00-09.50	<u>Pleneray talk</u>	
	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	