



AUTUMN SCHOOL:

CATALYSIS FOR EUROPE'S GREEN TRANSITION: ADVANCING INDUSTRIAL CATALYSIS BY SYNERGY OF EXPERIMENTS AND SUPERCOMPUTING SIMULATIONS

November 21-24, 2022

The school is organised in partnership with PRACE



TENTATIVE PROGRAMME

Venue: Conference Hall, Institute of Electrochemistry and Energy Systems, BAS, Acad. Georgi Bonchev Str., Bl. 10, 1113 Sofia

DAY 1: Monday, 21 November 2022

Morning session

09:15 – 09:45	Registration
09:45 – 10:00	Welcome address – Ilian Todorov, STFC UKRI, UK
10:00 – 11:00	Opening lecture: Richard Catlow, RS, UK
11:00 – 11:30	<i>Coffee break</i>

PART 1: TYPES OF CATALYTIC PROCESSING AND APPLICATIONS

11:30 – 12:15 Highlights on the contemporary hydrogen production technologies, Evelina Slavcheva, IEES – BAS, BG

12:15 - 13:30 *Lunch*

Afternoon session

13:30 – 14:15 Catalytic technologies for hydrogen production and purification, Tatjana Tabakova, IC-BAS, BG

14:15 – 15:00 Studies of adsorbed compounds using IR spectroscopy. Adsorption of CO₂ in porous materials, Konstantin Hadjiivanov, IGIC- BAS, BG

15:00 – 15:30 *Coffee break*

15:30 – 16:15 Designing new electrocatalytic materials for alkaline water splitting – challenges and prospective Ilia Valov, FZ Julich, Germany

16:15 – 17:00 PEM water electrolysis, Dimitrios Tsiplakides, Aristotle University of Thessaloniki, Greece

DAY 2: Tuesday, 22 November 2022

Morning session

09:30 – 10:15 Electrocatalysis in Fuel cells, Plamen Atanasov, University of California, Irvine, USA

10:15 – 11:00 Oxygen Reduction Reaction Electrocatalysis in neutral media - role of inorganic catalysts, enzymes and bacteria, Carlo Santoro, University of Milano-Bicocca, Italy

11:00 – 11:30 *Coffee break*

11:30 – 12:15 The electrochemical reforming for hydrogen production, Alessandro Lavacchi, ICCOM-CNR, Italy

12:15 - 13:30 *Lunch*

Afternoon session

13:30 – 14:15 Core-shell electrocatalysts, Sotirios Sotiropoulos, Aristotle University of Thessaloniki, Greece (confirmed with option for online participation)

14:15 – 15:00 SOEC and more complex catalysis at lower temperature, Peter Holtappels, Karlsruhe Institute of Technology, IT, Germany

15:00 – 15:30 *Coffee break*

15:30 – 16:15 Photocatalysis. Photocatalytic properties of TiO₂ and N, B N doped its nanotubes arrays, Stefan Armjanov, IPH - BAS, BG

16:15 – 17:00 Multi-method characterization and multi-scale modelling of catalysts for photoelectrochemical water splitting, Martin Bojinov, UCTM, BG

DAY 3: Wednesday, 23 November 2022

Morning session

09:30 – 10:30 Biocatalysis / Enzymatic Reactions, Adrian Mulholland, UoB, UK (on-line)

10:30 – 11:15 Electrochemically active biofilms of gram-positive and gram-negative bacteria applied as biocatalysts in bioelectrochemical systems, Jolina Hubenova, IEES – BAS, BG

11:15 – 11:30 *Coffee break*

11:30– 12:00 Q&A Session / Panel discussion

12:00 – 12:15 Closing remarks (Richard Catlow to be asked)

12:15 - 13:30 *Lunch*

PART 2: COMPUTATIONAL CATALYSIS

Afternoon session

13:30 – 14:15 Introduction to the ab-initio molecular dynamics and Metadynamics, Petko Petkov, UoS, BG

14:15 – 15:00 Introduction to the metal-organic frameworks (MOF) and their application in catalysis. Petko Petkov, UoS, BG

15:00 – 15:30 *Coffee break*

15:30– 16:15 Computational modelling of defects in porous materials. Petko Petkov, UoS, BG

16:15– 17:00 ML Studies of Catalysts, Albert Bruix, University of Barcelona

DAY 4: Thursday, 24 November 2022

Morning session

09:30 – 10:30 Basics of Quantum Chemical Methods, Georgi Vayssilov, UoS, BG

10:30 – 11:15 DFT modelling of the structure and the catalytic properties of transition metal nanoparticles and surface models, Hristiyan Aleksandrov or Iskra Koleva, University of Sofia

11:15 – 11:30 *Coffee break*

11:30 – 12:15 DFT modelling of the structure and the catalytic properties of metal oxides, Iskra Koleva or Hristiyan Aleksandrov, University of Sofia

12:15 - 13:30 *Lunch*

Afternoon session

13:30 – 14:15	Introduction to QM/MM modelling via ChemShell, Thomas Keal, UKRI STFC, UK
14:15 – 15:00	Demonstration of a ChemShell case study, Kakali Sen, UKRI STFC, UK
15:00 – 15:30	<i>Coffee break</i>
15:30 – 16:15	Computational modelling of zeolites, Georgi Vayssilov, UoS, BG
16:15 – 17:00	What are the supercomputing challenges for computational materials modelling, Peicho Petkov, UoS, BG

SCHOOL END

17:00 – 18:00	Closing remarks and round table.
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