

Program of the workshop

Continuum modeling in energy applications

Thursday, January 26, 2023, DIFFER, Eindhoven, the Netherlands

9.00 - 9.30	Registration	
9.30 – 9.45	Welcome and Opening	Marco de Baar, Director DIFFER Anja Biebere-Hütter, organizer of the workshop
9.45 – 10.20	Ulrike Krewer (keynote) Karlsruhe Institute of Technology, Germany	<i>Revealing limitations and potentials in electrosynthesis processes using micro- and macrokinetic modeling</i>
10.20 – 10.35	Nadav Snir Technion, Israel	<i>Calculating kinetic properties of surface reactions using wave propagation methods</i>
10.35 – 10.50	Bart van den Boorn DIFFER Eindhoven, the Netherlands	<i>Microkinetic and charge carrier transport modeling of the oxygen evolution reaction</i>
10.50 – 11.15	Coffee break	
11.15 – 11.50	Sebastian Matera (keynote) Fritz Haber Institute Berlin, Germany	<i>Bridging between electronic structure and continuum scales for heterogenous catalysis</i>
11.50 – 12.05	Tomasz A. Wesolowski Université de Genève, Switzerland	<i>Hohenberg-Kohn theorems as a basis for multi-scale simulations combining atomic and continuum representation of condensed matter</i>
12.05 – 12.20	Bastiaan Braams CWI, Amsterdam, the Netherlands	<i>Richly parameterized interaction potentials for atomistic modeling</i>
12.20 – 13.30	Lunch break and poster session	
13.30 – 14.05	Daniel Luder (keynote) RWTH Aachen University, Germany	<i>Data-driven parameter identification of an electrochemical model for Lithium-ion batteries with artificial intelligence</i>
14.05 – 14.20	Nigel Clarke University of Sheffield, UK	<i>Predicting structure/property relations in excitonic photovoltaic devices</i>
14.20 – 14.35	Seyedali Atyabi VITO, Belgium	<i>Electrochemical simulation of Alkaline Water Electrolyzer cell by 1D model with two different types of a membrane (Anion exchange membrane and separator)</i>
14.35 – 14.50	Mihai Butolo UPB Bucharest, Romania	<i>Photoelectrochemical water splitting using machine learning</i>
14.50 – 15.15	Coffee break	
15.15 – 15.30	Mykola Isaiev Université de Lorraine, France	<i>Atomistic simulations of energy transport across the solid/liquid interfaces</i>
15.30 – 15.45	Radhey Shayam Yadav Ariel University, Israel	<i>Tri-metallic alloys as an electro-catalyst for fuel cells – The case of MF on Pt3Pd3Sn2</i>
15.45 – 16.00	Klemen Bohic University of Ljubljana, Slovenia	<i>Surface charge characterization of nanoparticles</i>
16.00 – 16.30	Panel discussion with keynote speakers	
16.30 – 17.00	Closing with drinks	
18.30	Dinner in Eindhoven (optional)	