ÚFE Ústav fotoniky a elektroniky
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Computational Approaches to Catalyst Discovery for Urea Electrosynthesis

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This presentation reviews electrochemical co-reduction of CO_2 and nitrogen-containing species, which offers a sustainable route to urea, the world's most widely used fertilizer, using renewable electricity [1–4]. This approach presents a promising alternative to the energy-intensive Bosch–Meiser process. However, selective urea formation remains challenging due to complex multi-electron pathways and competing side reactions, making it difficult to simultaneously achieve high activity and selectivity.

Density functional theory (DFT) provides a powerful framework to address these challenges by enabling atomic-scale insight into reaction mechanisms and catalyst behaviour. In this talk, I will focus on identifying the key factors that govern catalyst performance for electrochemical C–N coupling. Using DFT, we investigate the co-reduction of NO_2^- and CO_2 to uncover the mechanistic origins of C–N bond formation [5]. Our results reveal an intrinsic activity–selectivity trade-off on pure metal surfaces, arising from the competing requirements for stabilizing key intermediates. These findings provide design principles for tuning adsorption energetics and catalyst composition to overcome these limitations and enable more efficient urea synthesis.

Speaker's profile

Dr. Mohammadreza Karamad is an Assistant Professor in the Chemistry and School of Sustainable Energy Engineering at Simon Fraser University. He holds a PhD in Physics from the Technical University of Denmark (DTU), an M.Sc. in Physics from the University of Tabriz, and a B.Sc. in Physics from Isfahan University of Technology. Prior to his current role, he served as an Assistant Professor in Physics and Astronomy at the University of Calgary and as a Research associate in chemical engineering there. His professional experience also includes industrial work as a materials design engineer in the USA and postdoctoral research at Stanford University. His research focuses on computational materials design using Density Functional Theory and Machine Learning. Applications include catalyst design for diverse electrochemical reactions for fuel and chemical synthesis and the development of advanced materials for energy technologies such as hydrogen storage.