KEMIJSKI INŠTITUT

Vabilo na Preglov kolokvij / Invitation to the Pregl colloquium


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## Četrtek / Thursday 17. 11. 2022, ob / at 13:00

Velika predavalnica Kemijskega inštituta /
Great Lecture Hall
National Institute of Chemistry
Hajdrihova 19, Ljubljana, Slovenia

# Multi-scale simulations of electrochemical energy storage systems


Progress in the development of energy storage systems is hampered by our lack of understanding of the microscopic mechanisms that determine their performance. The key issue is that phenomena on the atomistic scale have consequences on macroscopic properties. In particular, the effects of ionic confinement and diffusion are crucial for device performance, yet experiments that probe such properties locally are challenging and difficult to interpret. Here, I will focus on carbon-carbon supercapacitors which store energy through ion adsorption at the electrode surface. To understand such systems, it is essential to characterise finely the materials used and the properties of the fluid adsorbed. However, in order to screen materials, computationally efficient methods are needed. I will present insights from two approaches: i) molecular simulations which provide a microscopic understanding of the charging mechanisms and ii) a mesoscopic model we develop, 10,000 times faster than molecular simulations, for the prediction of electrochemical performance.


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Vljudno vabljeni / Kindly invited