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in kemijsko tehnologijo

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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

Understanding reactivity and electrochemical effects at interfaces from ab initio calculations

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Vljudno vabljeni!

Abstract:

Interfaces are fundamental to understand electrochemical reactions either for energy conversion applications (fuel cells), corrosion, electroplating or for electrochemical energy storages devices such as Li-ion batteries. Nevertheless, they are extremely complex to model because of the occurring electrochemical effects, but also because of the complexity of the electrode-solvent interface. Classical models reproduce the global behavior of such an interface fairly well, but they are oblivious to the quantum phenomena occurring at the interface. Ab initio approaches can describe this quantum behavior with good accuracy, nevertheless most of these approaches are not accounting for the full complexity of the electrochemical interface as it would necessitate including the solvent (at least hundreds/thousands of molecules) and electrolytes in their structural and time-dependent dimension leading to too costly calculations.
We will present an overview of interface calculations and reactivity rationalization and their extension to electrochemical interfaces modeling. We will first give some insights into surface reactivity and then extend the concepts to electrochemical reactivity by using specific tools such as a conceptual DFT approach: among many descriptors such as Density of State, electronic density variation etc., the Fukui function appears naturally for electrochemistry and gives direct information on the electrochemical processes.