

Universitatea din București, Facultatea de Chimie

Departamentul de Chimie Organica, Biochimie si Cataliza

Vă invită **13 Iunie, 2018, 14:00 – sala SP2 (Camin Panduri)** – la seminarul intitulat:

“Calculations of Product Selectivity in Electrochemical CO₂ Reduction”

susținut de:

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Faculty of Physical Sciences and
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Abstract:

CO₂ can be reduced electrochemically to form valuable chemicals such as hydrocarbons and alcohols using copper electrodes, whereas the other metal electrodes tested so far mainly form CO or formate, or only the side product, H₂. Accurate modeling of electrochemical reaction rates including the complex environment of an electrical double layer in the presence of an applied electrical potential is challenging. Calculated rates, obtained using a combination of density functional and rate theory, are in close agreement with available experimental data on the formation of the various products on several metal electrodes and over a range in applied potential, thus demonstrating the applicability of the theoretical methodology. The results explain why copper electrodes give a significant yield of hydrocarbons and alcohols, and why methane, ethylene, and ethanol are formed in electroreduction rather than methanol, which is the main product when H₂ gas reacts with CO₂ on copper catalyst. The insight obtained from the calculations has been used to develop criteria for identifying new and improved catalysts for electrochemical CO₂ reduction.