Electro-catalysis at the atomic scale

Prof. Jan Rossmeisl

University of Copenhagen, Denmark

Abstract :

The chemical industry should in the future be based on renewable energy. Therefore, material development for environmentally friendly, electrocatalytic production of valuable chemicals is needed. Chemicals could be produced using safe, cheap, more environmentally friendly and more abundant reactants than today. The products could be provided on demand at the place where they are needed, reducing expensive and hazardous transport of chemicals. However, stable, efficient and selective catalysts have to be discovered. This requires insight into the surface chemistry at the atomic scale. Surface chemistry can be revealed based on density functional simulations. However, there are presently no atomic scale simulations or analysis that capture all the essential parts of the nature electrochemical interface. Thus the electrochemical solid/liquid interface represents one of the frontiers of atomic scale simulations. I will give examples where the insight from simulations might pave the way for rational discovery of new catalyst materials and new electrocatalytic processes for sustainable production of fuels and chemicals. Some examples are: oxygen reduction to H2O2, Oxygen evolution [2] and CO2 reduction reaction [3].

[1] Enabling direct H2O2 production through rational electrocatalyst design. Siahrostami, Samira; Verdaguer-Casadevall, Arnau; Karamad, Mohammadreza; et al. NATURE MATERIALS, 12, 1137-1143, 2013

[2] Beyond the top of the volcano? - A unified approach to electrocatalytic oxygen reduction and oxygen evolution. Busch, Michael; Halck, Niels B.; Kramm, Ulrike I.; et al NANO ENERGY, 29, 126-135, 2016

[3] Understanding activity and selectivity of metal-nitrogen-doped carbon catalysts for electrochemical reduction of CO2. Ju, Wen; Bagger, Alexander; Hao, Guang-Ping; et al. NATURE COMMUNICATIONS 8, 944, 2017.

Bio :

Jan Rossmeisl is Professor of theoretical chemistry at Department of Chemistry and the Nano-Science center at Copenhagen University. Before joining University of Copenhagen in April 2015, Jan was an Associate Professor and group leader for the theoretical catalysis group at Department of Physics at the Technical University of Denmark Jan holds master's (2000) and Ph.D (2004) degrees in physics from the Technical University of Denmark. Since 2007 supervisor of ~30 Ph.D and Post docs. Coauthor of ~160 publications in peer reviewed journals, co-inventor of 5 patents and co-founder of two startup companies. Research interests include: electrocatalysis, energy conversion, atomic scale simulations, rational interface design for catalysis.