UNIVERSITY OF OSTRAVA
FACULTY OF SCIENCE

DEPARTMENT OF PHYSICS

Chemical Physics Group

Tuesday, December 20th, 11:00AM
Room M 312, Chittussiho 10, Ostrava

Michal Bajdich

SUNCAT Center, CHE Department and SLAC National Laboratory, Stanford University, California, USA

Transition Metal-Oxide Catalysis

In this theoretical talk, I will review the fundamentals and underlying principles governing the catalytic reactions. Special focus will be on processes that enable sustainable, CO_2 neutral, energy conversion and storage, such as electro-chemical water-splitting, hydrogen-evolution reaction, and CO_2 and N_2 reduction reactions. Next, I will single out transition metal-oxide materials as the most important materials for the electro-chemical reactions under oxidizing conditions and I will highlight our recent applications to layered 3d-transition-metal oxides,[1] mixed multi-metal oxide alloys,[2] and nanostructured supported metal oxides.[3] I well elaborate on the challenges in identification of the experimental and theoretical structures and active sites under the reaction conditions. Finally, I plan to discuss computational challenges limiting the progress in transition metal-oxide catalysis related to density functional theory.

[1] Bajdich, et. al, JACS (2013, 10.1021/ja405997s), JACS (2015, 10.1021/ja511559d)

[2] Bajdich, et. al, Science (2016, 10.1126/science.aaf1525)

[3] Bajdich, et. al. Nature Energy (2016, 10.1038/nenergy.2016.53), Nature Comm. (2016)