Skoltech
Skolkovo Institute of Science and Technology

When: Wednesday, Jul 17, at 16:00-17:00
Where: Skoltech, Blue Bldg, room 408

Computational Materials Science Seminar:

PREDICTIVE MODELING OF CHEMICAL REACTIONS IN HETEROGENEOUS CATALYSIS: TOWARD PHYSICS-BASED REACTIVE FORCE FIELDS

Speaker:

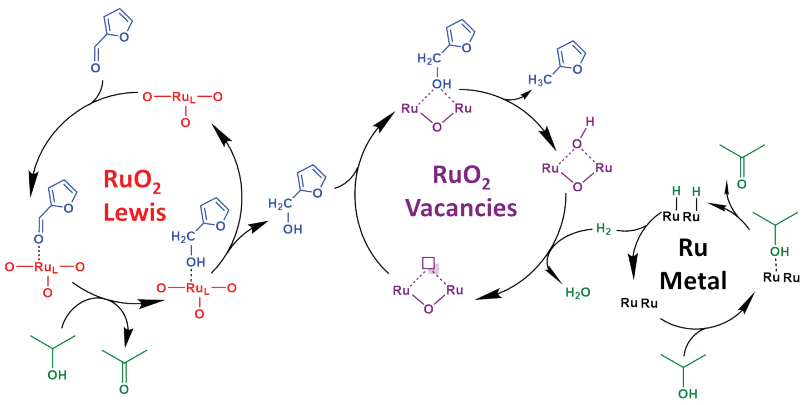
Dr. Alex Mironenko

Department of Chemistry of the University of Chicago, USA

ABSTRACT

Heterogeneous catalysts are essential ingredients for making 85-90% of the products of the chemical industry. Elucidation of catalysis by transition metal oxides with theoretical methods has been challenging due to inherent heterogeneity of their catalytically active surfaces and limitations of available quantum chemical methods. Nevertheless, a growing list of chemistries with the determinative role of initially present or in situ formed metal oxides necessitates urgent advancements in both their mechanistic understanding and quantum theoretical method development.

In the first part of my talk, I will focus on selective carbon-oxygen bond activation on a mixed Ru/RuO2 catalyst as a model chemistry relevant to renewable chemicals production and illustrate how first principles theoretical insights and microkinetic modeling revealed a trifunctional catalytic mechanism, consistent with every aspect of available experimental data. Based on mechanistic understanding, I will highlight theory-inspired principles of simultaneous design of the metal oxide catalyst and the reaction substrate and demonstrate their applicability to the seemingly unrelated areas of bimetallic and single-atom catalysis. Complexities in heterogeneous catalysis motivate the development of accelerated methods ("reactive force fields") to traverse configuration spaces in a computationally efficient manner. In the second part of the talk, I will describe a strategy to derive a reactive force field from first principles, by simplifying Kohn-Sham DFT equations through the application of the Weeks-Anderson-Davidson chemical pseudopotential theory. The resulting method shows promising, and to some extent, unexpected accuracy and transferability for model molecules composed of Group 1 elements. To the best of our knowledge, this is the first example of the topological and spin parameter transferability, exhibited by a semiempirical reactive potential.



BIOGRAPHY

Alex Mironenko graduated from the Chemistry Department of the Omsk F.M. Dostoevsky State University with honors in 2009, majoring in Chemical Engineering. He was awarded the Fulbright Fellowship to pursue the Master's Degree in Chemical Engineering at the University of Kansas in the area of experimental heterogeneous catalysis, which he obtained in 2012. In 2018, he got a Ph.D. in Chemical Engineering from the University of Delaware, working in the area of computational heterogeneous catalysis (Thesis title: "Untangling Complexities of Selective Carbon-Oxygen Bond Activation Using Multiscale Modeling and Quantum Theory Development"). His doctoral work has been recognized by the Achievement award of the Energy Frontier Research Center and the Allan P. Colburn Award.

Dr. Mironenko is currently a Kadanoff-Rice postdoctoral scholar at the Department of Chemistry of the University of Chicago. His research interests include elucidating reaction mechanisms in heterogeneous catalysis, development of physics-based and minimally empirical reactive force fields, and coarse-grained molecular dynamics.

LOOKING FORWARD TO SEEING YOU!

skoltech.ru/en