

Colloquium

Department of Engineering
and System Science,
Institute of Nuclear
Engineering and Science,
National Tsing Hua University

Understanding and design of catalysts on the nanoscale

Prof. Sergey Kozlov,
Assistant Professor,

**Department of Chemical and
Biomolecular Engineering,
National University of Singapore**

In the last decade, atomic simulations have become an important part of studies aimed at the understanding and design of new materials for catalysis, batteries, optoelectronic, structural, and other applications. In particular, atomic simulations have proven to be a valuable tool for studies of nanocomposite materials whose understanding requires precise atomic-scale characterization of their structure. Although resolving the 3D structure of nanocomposites often remains challenging in the experiment, the desired space and time resolution can be easily achieved in modern simulations.

This talk will describe our recent achievements in the understanding of nanocomposite properties using density functional (DFT) methods and overcoming various methodological challenges for such studies. For example, I will discuss how simulations enable the rational design of alloy nanoparticles whose composition and properties can be precisely tuned for optimal performance in a given application. Also, I will present our recent studies aimed to understand how strong interactions in nanocomposites composed of transition metal nanoparticles on oxide supports or oxide films supported on metal surfaces yield materials with atoms in unusual charge states as well as unique electronic and catalytic properties.

15:30-17:20 P.M., Wed., Oct. 5th, 2022
Synchronize online talk

Biography:



Education:

Postdoc at King Abdullah University,
Saudi Arabia (2016-2019)

PhD. at University of Barcelona, Spain
(2010-2015)

M.S. at Novosibirsk State University,
Russia (2007-2009)

B.S. at Novosibirsk State University,
Russia (2003-2007)

Selected Publications :

1. Knebel, Bavykina, Datta, Sundermann, Garzon-Tovar, Lebedev, Durini, Ahmad, **Kozlov**, Shterk, Karunakaran, Carja, Simic, Weilert, Klüpel, Giese, Cavallo, Rueping, Eddaoudi, Caro, Gascon. Solution processable metal-organic frameworks for mixed matrix membranes using porous liquids, *Nat. Mater.* 2020, 19, 1346.
2. Zhang, Wang, Cao, **Kozlov**, García de Arquer, Dinh, Li, Wang, Zheng, Zhang, Wen, Voznyy, Comin, De Luna, Regier, Bi, Alp, Pao, Zheng, Hu, Ji, Li, Zhang, Cavallo, Peng, Sargent. High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. *Nat. Catal.* 2020, 3, 985.
3. Wang, Cao, Zheng, Zhang, **Kozlov**, Chen, Zou, Kong, Wen, Liu, Zhou, Dinh, Zheng, Peng, Zhao, Cavallo, Zhang, Sargent. Hydration-Effect-Promoting Ni-Fe Oxyhydroxide Catalysts for Neutral Water Oxidation. *Adv. Mater.* 2020, 32, 1906806.
4. Suchorski, **Kozlov**, Beshpalov, Datler, Vogel, Budinska, Neyman, Rupprechter. The role of metal-oxide interfaces for long-range metal particle activation during CO oxidation. *Nat. Mater.* 2018, 17, 519.
5. Lykhach, **Kozlov**, Skála, Tovt, Stetsovych, Tsud, Dvořák, Johánek, Neitzel, Mysliveček, Fabris, Matolín, Neyman, Libuda. Counting electrons on supported nanoparticles. *Nat. Mater.* 2016, 15, 284.

Research Area:

- Density Functional Theory
- Modeling of Nanostructured Materials
- Computational Design of Materials for Catalysis and Electrochemistry

sergey.kozlov@nus.edu.sg