PHYSICAL CHEMISTRY 2021

4th International Meeting
on

Materials Science for Energy Related Applications

BOOK OF ABSTRACTS

September 22-23, 2021
University of Belgrade - Faculty of Physical Chemistry, Belgrade

UNIVERSITY OF BELGRADE
FACULTY OF PHYSICAL CHEMISTRY
Belgrade, Serbia

THE SOCIETY OF
PHYSICAL CHEMISTS OF SERBIA
Belgrade, Serbia

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Belgrade, Serbia

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in co-operation with

THE SOCIETY OF PHYSICAL CHEMISTS OF SERBIA

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Prof. Dr. Igor A. Pašti

Assist. Prof. Dr. Ana S. Dobrota

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DATA SCIENCE AND DEEP LEARNING FOR THE DEVELOPMENT OF NEW HYDROGEN STORAGE MATERIALS

Katarina Batalović, Jana Radaković, Bojana Paskaš Mamula

Laboratory of nuclear and plasma physics, VINCA Institute of nuclear sciences – national institute of the Republic of Serbia, University of Belgrade, Belgrade, Serbia

Prediction of metal hydride formation enthalpy is one of the key requirements for a rapid design of new hydrogen storage materials. In the last decades, DFT (density functional theory) approach showed good predictive potential for the ground state properties and accurate energies of hydride formation. However, calculating ZPE contribution and temperature effects in addition to formation energy at 0K is computationally and time-consuming and therefore often avoided, resulting in discrepancy to experiment.

The development of machine learning and, in particular, deep learning, opens a new perspective for predictive modeling of materials properties. Data collected through DFT calculations can be combined with experimental results in a predictive model, aiming to exploit unexplored compositional space. In this work, we consider the application of MatErials Graph Network (MEGNet) [1] to the prediction of hydrogen formation behavior, and screening of potential dopants in reversible metal hydride materials. Various approaches, relying on transfer learning and both experimental data and computational repositories (MP [2], NOMAD [3]) are proposed as a route to accurate prediction of a structure-property relation for hydrogen storage materials. Domains of applicability of these models are addressed.

References:

[1] C. Chen, W. Ye, Y. Zuo, C. Zheng, S.P. Ong, Chemistry of Materials, 2019, **31**, 3564–3572.

[2] A. Jain, S.P. Ong, APL Materials, 2013, **1,** 011002

[3] C.Draxl, M.Scheffler, J. Phys.Matter, 2019, **2**, 036001