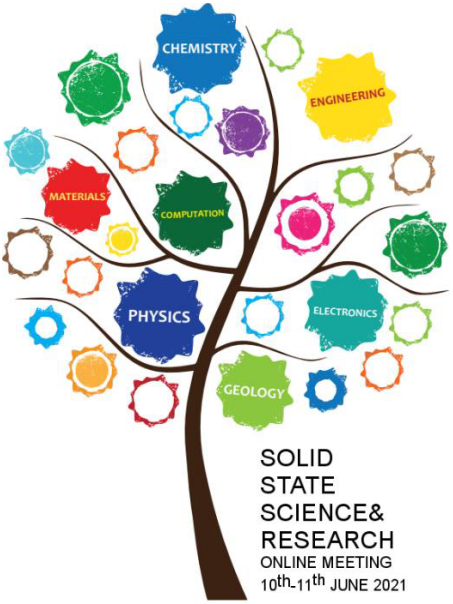
Book of Abstracts

10 & 11 June 2021, Zagreb, Croatia



Solid-State Science & Research
Zagreb, 10 & 11 June 2021

BOOK OF ABSTRACTS AND PROGRAMME

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Published by:

Ruđer Bošković Institute, Zagreb, Croatia

ISBN 978-953-7941-35-2

Published: *June 2021*

P33 - GNN and transfer learning for prediction of formation enthalpy of metal hydrides

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Prediction of metal hydride formation enthalpy is one of the key elements for a rapid screening and 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 calculation of hydride formation energies. Recently, graph neural network (GNN) implementations show promising results for fast and reliable prediction of formation energies for molecules and crystals. Here, we consider approach for universal machine learning based on a MatErials Graph Network (MEGNet) [1] that enable hydride formation energy prediction with a DFT accuracy. We demonstrate wide screening of potential dopants in Mg_2FeH_6 and Mg_2NiH_4. In addition, we study the potential of transfer learning for building the universal machine-learning model capable of addressing experimentally reported hydride formation enthalpies.

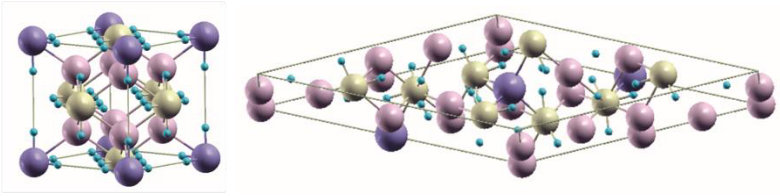

Figure 1 Unit cells of the doped Mg_2FeH_6 (left) and Mg_2NiH_4 (right)

[1] C.Chen, W.Ye, Y.Zuo, C.Zheng, S.P.Ong, *Chem. Mater.* **31** (2019) 3564.