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CONTEMPORARY BATTERIES AND SUPERCAPACITORS

INTERNATIONAL SYMPOSIUM BELGRADE 2022

PROGRAM AND BOOK OF ABSTRACTS

June 1-2, 2022,
Serbian Academy of Sciences and Arts
Belgrade, Serbia

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a) Батерије - Апстракти

Data-driven Design of New Mg-based Hydride Materials – A Synergy of Experiments and DFT

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Hydrogen absorption/desorption is one of the key processes underlying many clean energy applications, such as thermal energy storage, hydrogen storage, hydrogen compression, and nickel-metal hydride batteries. For all those applications fast and reliable characterization of new materials, and in particular, information regarding energetics of hydride formation reaction is of main interest. 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, MEGNet implementation [1] of graph neural networks showed promising results for fast and reliable prediction of formation energies for molecules and crystals. Here, we consider the development of a machine learning model based on the available DFT predicted structures and experimentally measured hydride formation enthalpies. The proposed model [2] is capable to predict hydride formation behavior for a wide variety of intermetallic compounds and distinguish the behavior of the polymorphs. In particular, based only on the crystal structure of the starting intermetallic compound, we were able to predict hydride formation enthalpy with accuracy comparable to DFT calculated values. Further, we demonstrate the application of this model for proposing new materials in Mg-Ni-M compound space with the desired enthalpy for hydrogen storage.

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[1] C.Chen, W.Ye, Y.Zuo, C.Zheng, S.P.Ong, Chem. Mater., Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals, 31 (2019) 3564.

[2] K.Batalović, J.Radaković, B.Paskaš Mamula, B.Kuzmanović, M.Medić Ilić, Predicting Heat of Hydride Formation by the Graph Neural Network – Exploring Structure-Property Relation for Metal Hydrides, preprint http://dx.doi.org/10.2139/ssrn.4055259

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The scientific man does not aim at an immediate result. He does not expect that his advanced ideas will be readily taken up. His work is like that of the planter — for the future. His duty is to lay the foundation for those who are to come, and point the way. He lives and labors and hopes.

Nikola Tesla

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