Artificial-intelligence assisted search for best energy-conversion materials

Sergey V. Levchenko[1]

[1]Skolkovo Institute of Science and Technology, Moscow 121205, Russia

Important properties of energy materials, such as activity and selectivity of a catalyst or a thermoelectric's figure of merit, are in general difficult to predict, in particular from first principles. The problem lies in the extreme complexity of the relation between the atomic composition of a material and its functional properties at realistic temperatures and pressures. We demonstrate how to bridge this complexity with artificial intelligence (AI) on several examples.

Single-atom metal alloy catalysts (SAACs) have recently become a very active new frontier in catalysis research. The simultaneous optimization of both facile dissociation of reactants and a balanced strength of intermediates' binding make them highly efficient and selective for many industrially important reactions. However, discovery of new SAACs is hindered by the lack of fast yet reliable prediction of the catalytic properties of the sheer number of candidate materials. We address this problem by applying a compressed-sensing approach SISSO parameterized with density-functional inputs. Besides consistently predicting high efficiency of the experimentally studied SAACs, we identify more than two hundred yet unreported candidates (Figure 1) [1].

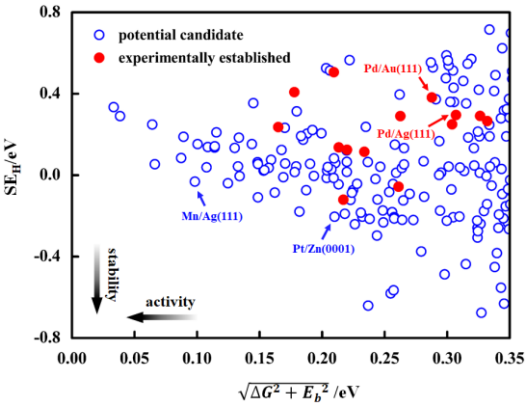

Figure 1. Stability vs. activity map for flat SAACs surfaces at T=298 K and p=1 atm.

Some of these candidates are predicted to exhibit even higher stability and efficiency than the reported ones. Our study demonstrates the importance of finding descriptors directly from data, as well as provides a recipe for selecting best candidate materials from hundreds of thousands of transition-metal SAACs for various applications.

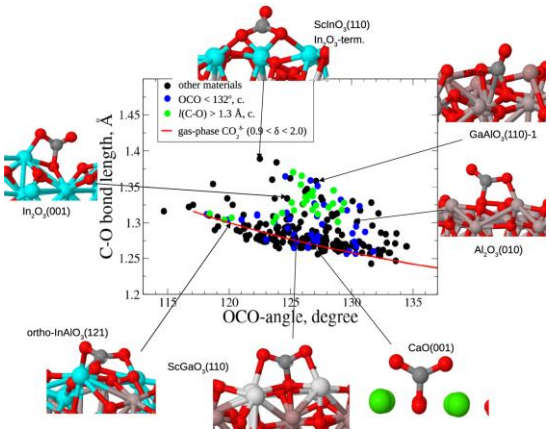

Figure 2. The OCO-angle in charged gas-phase CO2 is shown with the red line, and adsorbed CO2 structures are shown with the dots. The colored dots show the subgroups of best catalysts for two different mechanisms of CO2 activation.

Employing SISSO in an active-learning framework, we have also predicted and experimentally confirmed stable medium-temperature polycrystalline p-type thermoelectric (TE) materials with a very high figure of merit (~2). This breakthrough became possible due to the AI-assisted exploration of the vast materials space of a known class of TE materials, which allowed us to find materials with an optimal balance between conflicting parameters.

Moreover, using subgroup discovery, an AI approach that discovers statistically exceptional subgroups in a dataset, we develop a strategy for identification of most important parameters of a catalytic material and competing mechanisms of a catalytic reaction. The approach is used to develop physical understanding of hydrogen activation at SAAC's and address the problem of converting CO_2 to fuels and other useful chemicals (Figure 2) [2].

References

[1] Han, Z. K., Sarker, D., Ouyang, R., Mazheika, A., Gao, Y., & Levchenko, S. V. (2021). Nature Comm., 12(1), 1833.

[2] Mazheika, A., *et al*., (2022). Nature Comm., 13(1), 419.

Sergey V. Levchenko obtained M.Sc. from the Moscow Institute of Physics and Technology, and Ph.D. from Univesity of Southern California, LA, USA, in 2005. After a postdoc period at the University of Pennsylvania, PA, USA, he was a groups leader at the Fritz Haber Institute of Max Planck Society in Berlin, Germany, and since 2018 he is an assistant professor at Skoltech, Moscow, Russia. Sergey Levchenko is an expert in materials modelling using first-principles methods and artificial intelligence.

Presentating author: Sergey Levchenko, e-mail: s.levchenko@skoltech.ru tel: +79855703486