

# Comparison of machine learning strategies in the high-throughput exploration of $ABO_2$ delafossite oxides

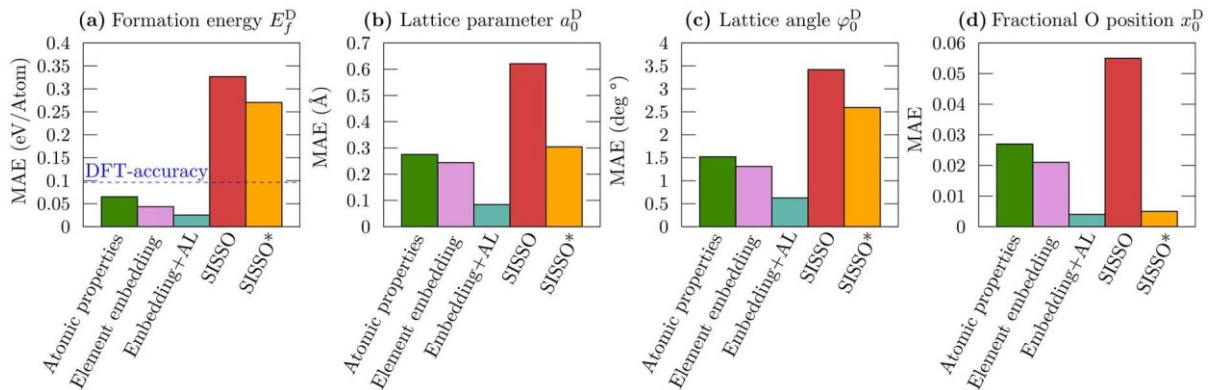
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The rise of machine learning introduced new computational techniques that promise to expedite the discovery of novel and possibly exotic materials. This raises a fundamental question about how these approaches balance interpretability versus accuracy. We address this aspect by comparing ensemble-based active learning of neural networks [1,2] and the *sure independence screening and sparsifying operator* (SISSO) [3] for the prediction of formation energies and lattice parameters in  $ABO_2$  delafossite oxides. To this end, we generate a consistent dataset from first principles. Element embedding is found to be superior to scalar input strategies, e.g., atomic properties. In conjunction with active learning, the neural networks rapidly reach DFT accuracy, allowing for a significant acceleration of high-throughput materials screening. In contrast, the precision of the physically interpretable SISSO descriptors is limited by the high data complexity. Moreover, we combine  $ABO_2$  infinite-layer,  $ABO_3$  perovskite [1,2], and the delafossite data to extend the unsupervised active learning approach into the structural space, thereby enhancing the sample efficiency in the spirit of transfer learning. Finally, we compile a phase diagram that compares the relative stability of these three distinct oxide materials classes.



[1] A. Sahinovic and B. Geisler, Phys. Rev. Research **3**, L042022 (2021)

[2] A. Sahinovic and B. Geisler, J. Phys.: Condens. Matter **34**, 214003 (2022)

[3] R. Ouyang *et al.*, Phys. Rev. Materials **2**, 083802 (2018)