Interpretable machine learning to understand and predict catalysts and materials

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Physically transparent and predictive models that quantify structure-property relationships of materials are important in many fields, including catalysis. Many of the high-profile applications of machine learning in catalysis and materials science have focused on using black-box models such as neural networks and Gaussian process regressors for the fast and accurate prediction of target properties such as material stability or adsorbate binding energies. Extracting meaningful physical insights from these black-box models has proven challenging, as the internal logic of these black-box models is not readily interpretable due to their high complexity. Interpretable ML methods that merge the predictive capacity of black-box models with the physical interpretability of physics-based models offer an alternative to black-box models. Interpretable models are desirable because they can lead to theories and hypotheses that advance our scientific knowledge and accelerate progress beyond solely enabling high-throughput screening.

In this talk, I will discuss three interpretable machine learning applications applied to various materials and catalysis problems. I will first present on using the Sure Independence Screening and Sparsifying Operator (SISSO) algorithm to find descriptors that predict the stability of perovskite oxides and halides.[1] SISSO finds a physically meaningful descriptor that predicts the stability of perovskite oxide and halide materials with superior performance compared to the well-known Goldschmidt tolerance factor. Second, I will present the use of supervised generalized additive models (GAMs) to clarify geometric structure-property relationships for chemisorption on metal alloys.[2] Third, I will show how unsupervised principal component analysis (PCA) can be used to establish relationships between the geometric structure, electronic structure, and chemisorption strength of adsorbates on alloys. By comparing the GAM-derived chemisorption models and the PCA analysis to previously established electronic-structure models, we clarify the critical physical parameters that control the chemisorption process on metal and alloy surfaces.

[1]. New tolerance factor to predict the stability of perovskite oxides and halides, C. J. Bartel, C. Sutton, B. R. Goldsmith, R. Ouyang, C. B. Musgrave, L. M. Ghiringhelli, M. Scheffler, *Sci. Adv.* 5, eaav0693 (2019).

[2]. Theory-guided machine learning finds geometric structure-property relationships for chemisorption on subsurface alloys, J. Esterhuizen, B. R. Goldsmith, S. Linic, *Chem* 6, 1 (2020).

[3]. Uncovering electronic and geometric descriptors of chemical activity for metal alloys and oxides using unsupervised machine learning, J. A. Esterhuizen, B. R. Goldsmith, S. Linic, *Chem Catalysis* 1, 1 (2021).