MACHINE LEARNING IN SURFACE SCIENCE AND CATALYSIS

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Recently developed machine learning methods hold great promise for simultaneously reducing the computational cost and increasing the accuracy in catalysis modeling, allowing us to capture more complexity, make our models more realistic and perhaps even obtain new physical insights. I will introduce our work using the compressed sensing "SISSO" method to develop physics-inspired and interpretable models for the binding energies of atoms and small molecules at various types of facets and active site motifs present at transition metal alloys and doped transition metal oxides [1-3]. Additionally, I will discuss recent work aimed at describing more complex adsorbates with bi- or polydentate adsorption motifs at transition metals and their alloys [4].
Further insights into the catalytic function of materials can be obtained by coupling density functional theory calculations (or machine learning predictions thereof) with kinetic models. I will show examples of varying complexity ranging from materials screening using inexpensive mean-field models [5] to a detailed investigation of CO hydrogenation over Rh catalysts, employing more computationally demanding kinetic Monte Carlo simulations in combination with cluster expansion techniques to treat adsorbate-adsorbate interactions [6].

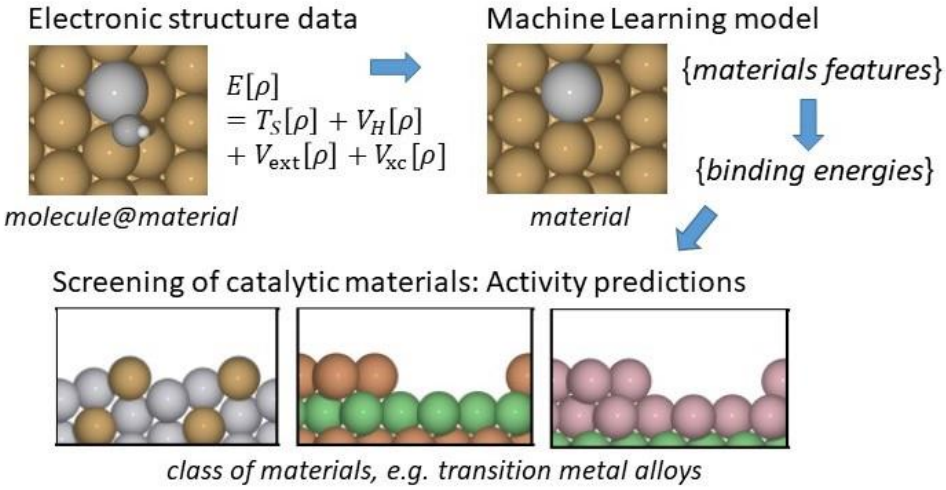

Figure 1: Machine learning models are developed to capture the relationship between materials features and binding energies of adsorbates, then serve as input for kinetic models used in materials screening.

[1] M. Andersen, S. Levchenko, M. Scheffler, and K. Reuter, *ACS Catal.* **9**, 2752 (2019).
[2] W. Xu, M. Andersen, and K. Reuter, *ACS Catal.* **11**, 734 (2021).
[3] M. Andersen and K. Reuter, *Acc. Chem. Res.* **54**, 2741 (2021).
[4] W. Xu, K. Reuter, and M. Andersen (*in preparation*).
[5] M. Deimel, K. Reuter, and M. Andersen, *ACS Catal.* **10**, 13729 (2020).
[6] M. Deimel, H. Prats, M. Seibt, K. Reuter, and M. Andersen (*in preparation*).