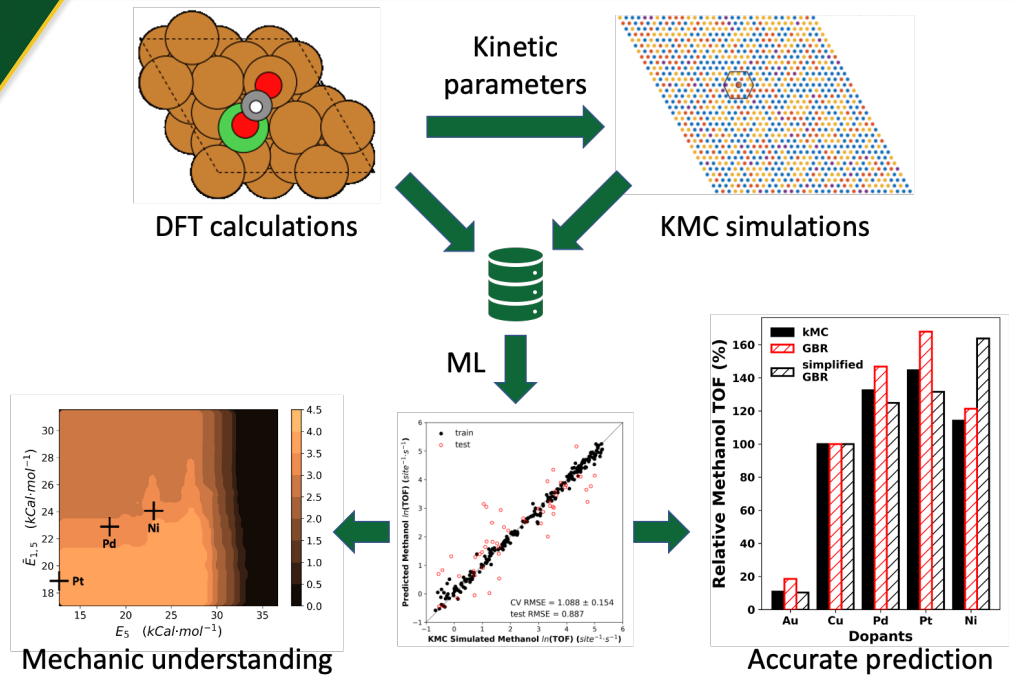
Data-driven Catalytic Descriptor Identification and Mechanism Understanding



Schematic for the proposed data-driven framework, a case study of identifying and interpreting activity-controlling descriptors in CO hydrogenation to methanol over Cu-based alloys.

W. Liao, P. Liu. *Catal. Sci. Technol.*, **2022**, DOI: 10.1039/D2CY00284A

The calculations was performed using the computing resources at the Center for Functional Nanomaterials, Brookhaven Nation Laboratory and the National Energy Research Scientific Computing Center.

Scientific Achievement

A data-driven machine learning (ML) framework was developed to predict the catalytic behaviors based on descriptors accurately and insightfully.

Significance and Impact

Accurate descriptor identification and performance prediction is of great important, but challenging in catalysis. The developed ML framework captures the non-local behaviors using the normalized second-order descriptors and demonstrates higher accuracy and efficiency to predict catalytic activities than the typical derivative-based methods.

Research Details

- ML surrogate model enabled identification of effective descriptors and accurate prediction of catalytic activity.
- Model-agnostic interpretation method unraveled the role of descriptors and promoted the mechanic understanding of reaction kinetics.