Atomic structure-free representation of active motifs for expedited catalyst discovery

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In computational catalysis, binding energies of reaction intermediates are important descriptors to predict catalytic activities and discover new catalyst using density functional theory (DFT) calculations. Recently, machine learning have been used to reduce the number of computationally intensive DFT calculations for a high-throughput screening. However, to predict binding energy of new materials, these methods require several steps, such as structure optimization and modeling. In this work, we report an atomic structure-free representation of active motifs to predict binding energies, which could bypass the time-consuming processes in the conventional approach. For training the model, we identify active site atoms and their nearest neighboring atoms positioned in the same layer and sublayer, and atomic properties are collected to construct input fingerprints. Our method predicted CO and H binding energies with high accuracy. Furthermore, our method can generate new active motifs without any DFT calculations, predict their binding energies and validate prediction results. The predicted binding energy distributions can suggest promising candidates to accelerate catalyst discovery.