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Scaling Relationships across Chemically Related Adsorbates for Fast Screening of Alloy Catalysts for Propane Dehydrogenation

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ABSTRACT

A catalyst is a material which speeds up the rate of a specific reaction. A reaction that is of significant importance to the chemical industry is the selective transformations of light alkanes (ethane, propane), which are largely available in shale gas, to olefins. These olefins can then be converted into higher-value chemicals, materials, and fuels. However, there are several undesired reactions that take place alongside the main dehydrogenation reaction, so a catalyst of high selectivity is desired. Apart from the industrially used PtSn catalyst, work by our experimental collaborators has shown that various other Pt and Pd alloys (In, Zn) are also highly selective and active for propane dehydrogenation (PDH). We aim to use Density Functional theory (DFT) to determine the trends in catalytic reactivity and selectivity across a wider space of alloy catalysts. This can be achieved through the development of linear scaling relationships (LSR), which relate the thermodynamic adsorption properties of chemically related species on various alloys. Initial results on the Pd alloys (Pd3Sn, PdIn, PdZn) show that the alloys have lower binding energies as compared to a pure metal. These results can have implications on the higher selectivity observed on the alloys experimentally.

KEYWORDS

Catalyst, dehydrogenation, Density Functional Theory, scaling relationships, alloys, reactions