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Probing and modeling orbital-specific contributions to chemisorption using DFT SARA E. MASON, ILYA GRINBERG, ANDREW M. RAPPE, University of Pennsylvania — We present a DFT study of atomic and molecular chemisorption spanning a variety of transition metals, facets and adsorption geometries. We cast our results in a physical model for chemisorption that takes into account which metal and adsorbate orbitals interact to form chemisorption bonds. We use DFT chemisorption energies, orbital overlaps and changes in charge density induced by adsorption to track how the metal and adsorbate states interact as a function of metal identity, surface facet, adsorption geometry and strain. We introduce strain to the adsorption systems as a probe that causes relatively small, but geometrically specific, changes to electronic structure of the metal. By taking into account orbital specific contributions to chemisrotpion, our model is able to reproduce subtle differences in chemisorption present in our DFT results and offers a means for predicting adsorption energies on different metal surfaces at different sites and in different states of strain.

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