

Abstract Submitted
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Evaluating DFT for Transition Metals and Binaries: Developing the V/DM-17 Test Set¹ ELIZABETH DECOLVENAERE, Univ of California - Santa Barbara, ANN MATTSSON, Sandia National Laboratories — We have developed the V-DM/17 test set to evaluate the experimental accuracy of DFT calculations of transition metals. When simulation and experiment disagree, the disconnect in length-scales and temperatures makes determining “who is right” difficult. However, methods to evaluate the experimental accuracy of functionals in the context of *solid-state materials science*, especially for transition metals, is lacking. As DFT undergoes a shift from a descriptive to a predictive tool, these issues of verification are becoming increasingly important. With undertakings like the Materials Project leading the way in high-throughput predictions and discoveries, the development of a one-size-fits-most approach to verification is critical. Our test set evaluates 26 transition metal elements and 80 transition metal alloys across three physical observables: lattice constants, elastic coefficients, and formation energy of alloys. Whether or not the formation energy can be reproduced measures whether the relevant physics are captured in a calculation. This is especially important question in transition metals, where active d-electrons can thwart commonly used techniques. In testing the V/DM-17 test set, we offer new views into the performance of existing functionals.

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