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Modeling Point Defects in Austenite using Density Functional Theory RON GIBALA, University of Michigan, WILLIAM COUNTS, CHRIS WOLVERTON, Northwestern University — Austenite is an fcc based, paramagnetic phase of iron that is an important component in many commercial steels. Modeling the paramagnetic state using DFT is problematic due to the disordered magnetic structure. Here, we use DFT to investigate the properties of pure and defected fcc Fe in a number of different (collinear) magnetic orderings in an effort to find a suitable model for austenite. We compare the properties of the following magnetic orderings: ferromagnetic, non-magnetic, and various anti-ferromagnetic arrangements. We investigate the formation and binding energies of vacancy, carbon, and hydrogen point defects in fcc Fe with each potential magnetic state. Where possible, experimental results were used as a metric to judge each magnetic phase. We find that an antiferromagnetic phase containing alternating double layers of spin up and spin down (AFM-DL) is the best surrogate for paramagnetism in austenite.

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