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First principle modeling of magnetic structure in Fe-C and intermetalics[1] AURELIAN RUSANU, DON NICHOLSON, ORNL, MARKUS EISENBACH, G.M. STOCKS, ORNL — Magnetic structure in Fe rich materials presents a high dependence on local atomic arrangement affecting mechanical, magneto-caloric, and magnetization properties. Insights into local properties and bulk effects can be obtained from first principle analysis. In this study we deploy the LSMS and VASP methods to model the ground states of various Fe-C systems. Behavior at finite temperature would be discussed in terms of diffusion barriers calculated by nudged elastic band method(VASP) and the energy of the magnetic fluctuations by constrained density functional theory (LSMS).

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