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First-principles studiesy of the order-disorder phase transition in FeCo using Wang-Landau Monte-Carlo method[1] ZONGRUI PEI, MARKUS EISENBACH, G. MALCOLM STOCKS, Oak Ridge National Lab — Simulating order-disorder phase transitions in magnetic materials requires the accurate treatment of both the atomic and magnetic interactions, which span a vast configuration space. Using FeCo as a prototype system, we demonstrate that this can be addressed by combining the Locally Self-consistent Multiple Scattering (LSMS) method with the Wang-Landau (WL) Monte-Carlo algorithm. Fe-Co based materials are interesting magnetic materials but a reliable phase diagram of the binary Fe-Co system is still difficult to obtain. Using the combined WL-LSMS method we clarify the existence of the disordered A2 phase and predict the Curie temperature between it and the ordered B2 phase. The WL-LSMS method is readily applicable to the study of second-order phase transitions in other binary and multi-component alloys, thereby providing a means to the direct simulation of order-disorder phase transitions in complex alloys without need of intervening classical model Hamiltonians. We also demonstrate the capability of our method to guide the design of new magnetic materials.

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