

Abstract Submitted
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Magnetic properties of Fe-based ferromagnets: a first-principles study¹ OLGA VEKILOVA, OLLE ERIKSSON, HEIKE HERPER, Materials Theory, Uppsala University — The increasing importance of permanent magnets to the modern society has resulted in renewed interest in the design of new magnetic materials that are cheap and abundant. A good permanent magnet must have a high Curie temperature, high saturation magnetization and uniaxial anisotropy energy. Fe-rich systems like the hcp Fe₃Sn compound are promising candidates. However, as it turned out to be an easy plane magnet. One of the possibilities for changing the easy axis direction is through alloying. Here we use theoretical modelling to discover new advanced permanent magnets. We study from first principles the electronic structure of Fe-based alloys, that exhibit ferromagnetic properties naturally, in combination with phase stabilizers, such as Sn, Sb, Ga, Ge and lighter elements such as Si and N in order to understand the origin of magnetic properties and find new ferromagnetic phases with uniaxial anisotropy that can be used for development of advanced permanent magnets. The stability of the phases is elucidated theoretically by the calculation of formation enthalpies. The trends in the calculated magnetocrystalline anisotropies and Curie temperatures of these compounds are analyzed and suggestions for the better permanent magnets are formulated.

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