

Materials Science and Technology Division

“Platinum and platinum compounds
modeling: From bulk to nano”

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Abstract:

Understanding the physics of the transition from bulk to nanoscale alloys is important from both a fundamental and a technological point of view. We present an ab-initio based theoretical study of both bulk and nano properties of platinum and a number of platinum compounds as they are promising materials for current and future technological applications in catalysis, ultrahigh-density magnetic recording, spintronics and high-performance permanent magnets. In particular, the ground state configurations of Fe-Pt alloy are estimated (using cluster expansion technique with structural and magnetic “filters”). The comparative study of FePt and MnPt magnetic properties is performed, showing that they may be considered as magnetic antipodes. The study of the size effect on the atomic structure of FePt nanoparticles indicates that the core’s ordered state is not affected by surface thermodynamics as much as previously thought. We show that addition of Au and Ag to FePt nanoparticle is not helpful for change of its structural state as Au and Ag additives tend to segregate from FePt (in contrast to Cu additives). An approach for prediction of stable and metastable shapes of nanoparticles as function of their size is developed. It is based on first principles calculation of high-index surface-energies and nanoparticle surface-tension excess free energies without phenomenological approximations. The approach is applied in the case of platinum nanoparticles. The theoretical predictions are verified by comparison with direct first principles calculations for small clusters.

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