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Structural defect properties of Co-Pt-type magnetic-storage alloys from an optimized basis-set representation[1] AFTAB ALAM, DUANE JOHNSON, University of Illinois at Urbana Champaign — Within a rapidly computed site-centered basis-set determined from the local saddle-points in the overlapping atomic charge densities, we shall describe an optimal respresentation which separate the "spherical" density and potential around an atom from the symmetry-induced, "non-spherical" interstitial part. These saddle-point radii (SPR) define the inscribed "muffin-tin" radii that determine uniquely the convex Voronoi polyhedra (VP) surrounding a site, thus more properly reflect the charge transfer, atomic size effects and hence the Energetics. We implement the idea of this SPR-basis within a first principles calculation to investigate the effect of thermal processing in several CoPt-type magnetic storage alloys. We predict accurately the stability of chemically and magnetically ordered and disordered phases, structural defects energies, as well as thermodynamic transformation temperatures in agreement with those of full-potential calculations and experiments.

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