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Role of defect coordination environment on point defects formation energies in Ni–Al intermetallic alloys EMRYS TENNESSEN, JAMES RONDINELLI, Northwestern Univ — We present a relationship among the point defect formation energies and the bond strengths, lengths, and local coordination environment for Ni–Al intermetallic alloys based on density functional calculations, including Ni_3Al, Ni_5Al_3, NiAl, Ni_3Al_4, Ni_2Al_3 and $NiAl_3$. We find the energetic stability of vacancy and anti-site defects for the entire family can be attributed primarily to changes in interactions among first nearest neighbors, owing to spatially localized charge density reconstructions in the vicinity of the defect site. We also compare our interpretation of the local coordination environment with a DFT-based cluster expansion and discuss the performance of each approach in predicting defect stability in the Ni–Al system.

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