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High through put computation of defect properties in metals BHARAT MEDASANI, MACIEJ HARANCZYK, Lawrence Berkeley Natl Lab, MARK ASTA, University of California Berkeley — We combine first principles density functional method and MPWorks, a high throughput framework, to compute the vacancy formation energies in metals. Three different exchange correlation (xc) functionals, PBE, PW91 and LDA are evaluated with respect to the computed formation energies. Bulk and defect structures are relaxed using a mesh of 108000 k-points X atoms to achieve an accuracy of 10 meV or better. Of the three functionals, LDA gives better results compared to the PBE and PW91 (GGA) functionals due to the cancellation of exchange and correlation errors arising due to the presence of internal void surface. PBE and PW91 predict noticeably different vacancy formation energy values even though the lattice constants and cohesive energies predicted by them are very close. Applying surface error correction brings the formation energies computed with the three functionals closer to the experimental values. The surface correction is in general small for LDA and bigger for GGA functionals. Meta-GGA functionals are expected to predict better surface energies and hence better vacancy formation energies. We report the performance of one such meta-GGA functional, revTPSS.

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