

Abstract Submitted
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Empirical potentials from a combined density functional theory / genetic algorithm approach: Illustration for Xe in UO₂ ALEXANDER THOMPSON, BRYCE MEREDIG, CHRIS WOLVERTON, Northwestern University — We have developed a new empirical potential for xenon in uranium dioxide with existing UO₂ potentials that achieves accurate xenon defect energetics. This potential was fit to several snapshots of DFT+U molecular dynamics of a single defect configuration using the genetic algorithm code Iterative Potential Refinement (IPR). In IPR, the forces, stresses, and energies from DFT calculations are used to parameterize empirical potentials. Several random sets of parameters are used to compare against DFT and the genetic algorithm minimizes the error of the parameters with respect to the DFT results. We compare this potential and other xenon potentials to DFT+U using a large set of defect calculations of xenon incorporated into sites with high, intermediate, low strain. Despite only being fit to a single configuration, our new empirical potential gives the very good agreement with DFT+U across a range of xenon incorporation sites and vastly outperforms existing xenon potentials.

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