Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Monovacancy Properties From Atomistic Simulations Based on OpenKIM[1] JUNHAO LI, JAMES SETHNA, Cornell Univ — A longtime goal of scientists is to be able to calculate the properties of materials from their structures accurately and efficiently. And atomistic simulation with good interatomic potentials has its unique position in the trade-off between these two targets. Different models may be suitable for different situations and our study focus on vacancy, the simplest and the most common point defects. In order to assess how each interatomic potential model performs in vacancy-related simulations, we calculate the most important monovacancy properties for all the elements and all the simple crystal structures predicted by the interatomic potential models available on OpenKIM at this time. These results can provide useful information for selecting interatomic models. We also examine how these properties depend on each other and other elemental properties. In particular, we shall report on relationships between the vacancy formation energy, the migration energy, the surface energy and the elastic constants, and how these relationships depend on the class of interatomic potential.

[1]NSF

Junhao Li
Cornell Univ

Date submitted: 02 Nov 2016 Electronic form version 1.4