

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**OpenKIM - Building a Knowledgebase of Interatomic Models**

MATTHEW BIERBAUM, Cornell University, ELLAD TADMOR, RYAN ELLIOTT, TREVOR WENNBLOM, University of Minnesota, ALEXANDER ALEMI, YAN-JIUN CHEN, Cornell University, DANIEL KARLS, ADAM LUDVIK, University of Minnesota, JAMES SETHNA, Cornell University — The Knowledgebase of Interatomic Models (KIM) is an effort by the computational materials community to provide a standard interface for the development, characterization, and use of interatomic potentials. The KIM project has developed an API between simulation codes and interatomic models written in several different languages including C, Fortran, and Python. This interface is already supported in popular simulation environments such as LAMMPS and ASE, giving quick access to over a hundred compatible potentials that have been contributed so far. To compare and characterize models, we have developed a computational processing pipeline which automatically runs a series of tests for each model in the system, such as phonon dispersion relations and elastic constant calculations. To view the data from these tests, we created a rich set of interactive visualization tools located online. Finally, we created a Web repository to store and share these potentials, tests, and visualizations which can be found at <https://openkim.org> along with further information.

Matthew Bierbaum  
Cornell University

Date submitted: 15 Nov 2013

Electronic form version 1.4