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Knowledgebase of Interatomic Models application programming interface as a standard for molecular simulations

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ABSTRACT

Nanoscale modeling of materials often involves the use of molecular simulations or multiscale methods. These approaches frequently use empirical (fitted) interatomic potentials to represent the response of the material. As part of the open Knowledgebase of Interatomic Models (KIM) project (https://openkim.org), an application programming interface (API) for interatomic potentials has been developed in consultation with key members of the materials simulation community. The KIM API is beginning to emerge as a standard for atomistic simulations of materials. This API makes it possible for any KIM-compliant (KIM API conforming) simulation code ("Simulator") to seamlessly use any KIM-compliant potential ("Model") obtained from https://openkim.org. The KIM API is also necessary for the KIM Processing Pipeline in https://openkim.org to automatically compute the predictions of stored Models for a variety of material properties by linking them to computer programs called "Tests" that perform these calculations. The KIM API is lightweight and efficient, supports physical unit conversion, a variety of common neighbor list and boundary conditions used in atomistic simulations, and provides multilanguage support for C++, C, Fortran 2003, Fortran 90/95, and Fortran 77, allowing Simulators and Models written in any of these languages to work together.