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Knowledgebase of Interatomic Models (KIM): Reliable Interatomic Models for Molecular Simulations

ABSTRACT:

Atomistic and multiscale simulations of materials using empirical interatomic potentials play a key role in realistic scientific and industrial applications. The Open Knowledgebase of Interatomic Models project (<https://OpenKIM.org>) [1,2] includes an automated user-extendable framework for testing the predictions of potentials for a host of material properties. Visualization tools have been developed to compare potential predictions to help select the most appropriate one for a given application. Verification checks ensure the integrity of the potentials. The potentials in OpenKIM conform to the KIM application programming interface (KIM API), which means that they can be seamlessly used with several major molecular simulation codes that support the KIM standard. This talk will describe the OpenKIM project and how the testing framework can assist materials researchers.



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BIOGRAPHY:

Ellad B. Tadmor is a Professor of Aerospace Engineering and Mechanics at the University of Minnesota (USA). He received his B.Sc. and M.Sc. in Mechanical Engineering from the Technion -- Israel Institute of Technology in 1987 and 1991, and his Ph.D. from Brown University (USA) in 1996. His research focuses on the development of multiscale theories and computational methods for predicting the behavior of materials directly from the interactions of the atoms making up the material. He has published over 60 papers in this area and two textbooks (see <http://modelingmaterials.org>). Prof. Tadmor is the Director of the Knowledgebase of Interatomic Models (OpenKIM.org) project which is tasked with developing standards for atomistic simulations and improving transferability of interatomic potentials. He was a Postdoctoral Research Fellow at Harvard University (USA), Associate Professor at the Technion (Israel), and Erasmus Mundus Scholar at the Ecole Normale Supérieure in Lyon (France). He received the MRS Graduate Student Award in 1995 for his work on developing the quasicontinuum method, one of the leading multiscale methods, as well as numerous awards for excellence in teaching including the Salomon Simon Mani Award in 2001. Prof. Tadmor is on the Editorial Board of the Journal of Elasticity.