KIM seeking candidates for an NSF fellowship in
"Transformative Computational Science using CyberInfrastructure" (CI TraCS)

Overview of KIM: Atomistic or molecular simulations of materials can play a key role in the development of innovative technologies that address important problems (including climate change, energy, and terrorism). To model the large numbers of atoms required for many applications, and to study their dynamics over reasonable time scales, approximate models of interatomic bonding, referred to as "interatomic potentials" or "interatomic models," are often used. Generally, these models define the forces and energies used in simulation methodologies such as molecular dynamics, Monte Carlo, multiscale methods, and so on. From such simulations, complex materials properties and phenomena can be extracted, including such things as melting temperatures, solid-liquid interface phenomena, fracture properties, and dislocation nucleation and motion.

KIM (http://openKIM.org) is a current initiative (lead by PI's: Ellad B. Tadmor, Ryan S. Elliott, and James P. Sethna) to develop and implement standards for the atomistic simulation of materials. The project aims to help bring order to the efforts of the education, research, and industrial communities and to make it easier for new (and existing) scientists to leverage the work of other in this important field. The KIM project has two main objectives:

1. Development of an online resource for standardized testing and long-term warehousing of interatomic potentials and data. This includes the development of *application programming interface* (API) standards for coupling simulation codes and interatomic potential subroutines.

2. Development of a quantitative theory of transferability of interatomic potentials to provide guidance for selecting application-appropriate models based on rigorous criteria and error bounds on results.

To learn more about the KIM project, visit http://openKIM.org and click on "About Us" and "Resources".

Overview of CI TraCS: The overarching goal of the NSF Fellowships for Transformative Computational Science using Cyberinfrastructure (CI TRaCS) program is to support outstanding scientists and engineers who have recently completed doctoral studies and are interested in pursuing postdoctoral activities in computational science, and thereby nurturing the future leaders in this emerging and important multidisciplinary field. Computational research and education activities that are cyberinfrastrucure-based and cross disciplinary boundaries are a key focus of this program. Successful Fellows may, for example, use cyberinfrastructure to make revolutionary advances in their disciplines, and/or deploy cyberinfrastructure-based technologies that enable innovative computational practices. (See http://www.nsf.gov/pubs/2010/nsf10553/nsf10553.htm for further information.) Note that CI TraCS applicants must be U.S. citizens, nationals or permanent residents.

Seeking candidates: The KIM PI's are seeking qualified postdoctoral candidates who are interested in applying to the NSF CI TraCS program. If selected by the KIM PI's, the successful candidate would work closely with the KIM PI's to develop a comprehensive and detailed CI TraCS proposal based on the needs and goals of the KIM project. The postdoctoral candidate would submit this proposal to NSF by the January 13, 2012 deadline. If NSF awards the candidate a fellowship, the fellow would be given a three-year (with the possibility of a fourth year, depending on availability of funds) appointment at the University of Minnesota, Twin-Cities Campus (Minneapolis, MN).

To Apply: Interested candidates should contact Ellad B. Tadmor (tadmor@aem.umn.edu) and provide (1) their CV, (2) a (one page or less) statement summarizing how their background, interests, and skills are a good fit with the KIM project, and (3) a list of three (or more) references. **Applications are due by November 14, 2011.**