Postdoctoral position – multi-scale modeling of complex materials

Massachusetts Institute of Technology (MIT), Department of Civil and Environmental Engineering (CEE)

We are currently seeking outstanding applicants for a postdoctoral position starting in fall 2005 in the area of multi-scale modeling and simulation. Applicants should have a doctoral degree in engineering, physics, chemistry, materials science or a related area. The research will be carried out in Dr. Buehler's lab at MIT in the Department of Civil and Environmental Engineering (CEE). This position is specifically targeted towards multi-scale modeling method development, in particular focusing on coupling of atomistic-mesoscale and atomistic-continuum scales including work on reactive potentials. The goal is to achieve coupling of first principles based reactive potentials to nonreactive, mesoscale and macroscale material theories to model complex chemistry and its relation to mechanical properties of materials (e.g. in stress corrosion cracking, or cracking of polymers). The ideal candidate should have good knowledge and experience in code and algorithm development (including C, C++, FORTRAN and preferably scripting languages such as Python). At the same time, we hope that the candidate has a strong background and interest in scientific issues related to multi-scale modeling and coupling of different scales. Expertise and familiarity using first principles MD, empirical MD, meso-scale or continuum-scale methods is essential.

Overall project description

It has always been the dream of computational scientists to understand the properties and behavior of materials based on computer simulation from a very fundamental perspective. Within the coming decade, this dream may come true and we will be able to predict macroscopic properties of complex materials throughout hierarchies of scales and paradigms. The key to achieve this is the availability of computational tools that allow straightforward integration of highly complex computational engines for materials simulations. We believe that paradigm complexity in materials modeling is essential to address important scientific problems, in particular those at the interfaces of different scientific disciplines as for example interfaces between living and non-living systems in hybrid nano-bio technologies. The development of our new multi-scale multi-paradigm simulation environment, the “Computational Materials Design Facility” (CMDF) is the realization of this vision and has been successfully applied to address critical problems in the behavior of materials including fracture, oxidation of surfaces, as well as modeling of biological systems. The method couples quantum mechanical (QM) methods, the new first principles ReaxFF reactive force field and empirical all atom force fields (FF).

This position involves further development of these multi-scale multi-paradigm simulation...
methods within our CMDF framework. Particular emphasis is given on integrating our new reactive force fields (ReaxFF), non-reactive force fields, mesoscale and continuum approaches. This will require development and application of novel algorithms, methods and interfaces to couple different paradigms across hierarchies of scales both in time and space. Applicants are expected to carry out cutting edge research at the interfaces of physics, chemistry, biology and materials science.

This project is a collaboration with the Materials and Process Simulation Center directed by Prof. William A. Goddard III, professor of chemistry, materials science, and applied physics at the California Institute of Technology, Pasadena CA.

Please send your application material in electronic form to:

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The application material should include:

- Curriculum Vitae.
- Brief statement of immediate and long-term research interest, not exceeding one page. Please include a description of how your background is appropriate for this opening.
- Research experience statement, no more than two pages. Please summarize your achievements and contributions.
- A complete listing of papers appearing in refereed publications or in conference proceedings, beginning with the most recent. Please include 2-3 representative publications in electronic form.
- A list of any academic honors or awards received.
- Please include addresses, positions and contact information of at least three references in your application material.

Salary and benefits

Salary is commensurate with demonstrated capabilities and experience. We offer an attractive benefits package. This position will involve an appointment as Postdoctoral Scholar at Caltech (in Prof. Dr. William A. Goddard’s lab in the Division of Chemistry), but the research will be carried out at MIT. Caltech is an equal opportunity employer.