

Two Postdoc Positions: DFT/MD and AFM of Oxide Interfaces

The School of Engineering and Applied Science at the University of Pennsylvania invites applications for two full-time Postdoctoral Researcher positions in the laboratories of Prof. D.S. Srolovitz (<https://www.seas.upenn.edu/directory/profile.php?ID=180>) and Prof. Robert W. Carpick (<http://carpick.seas.upenn.edu>).

These two positions are part of a multi-year, multi-institutional, interdisciplinary research effort on the development, characterization, and integration of materials for nano-electromechanical systems (NEMS) switch technology, funded by the National Science Foundation. The project involves close collaboration between computational materials scientists (DFT and MD) and experimentalists (materials scientists, mechanical engineers, electrical engineers). The project spans from first principles materials selection up to the fabrication of working NEMS devices.

The first position, to be supervised jointly by Professors David Srolovitz and Robert Carpick, is in the area of first principles modeling of interfaces, interfacial adhesion, and electrical conductance in metal oxides. This research focuses on DFT-based calculations of surface and interface properties in a wide-range of electrically conductive (e.g., semimetallic, semiconducting, point-defect mediated) metal-oxides (e.g., RuO₂, TiO_x, Ta₂O_x). This includes establishing DFT-based workflows for systematic screening of conductive metal-oxide structure and properties in order to develop effective heuristics for material selection (e.g., low adhesion, large conductance). The main tools are expected to be Quantum Espresso and VASP, as well as Boltzmann transport, Kubo-Greenwood and/or non-equilibrium Green's function (NEGF) approaches.

The successful applicant (recent PhD with or without prior postdoctoral study) should have experience in density functional theory-based approaches and transport methods in ceramics, metals and/or semiconductors.

The second position, to be supervised by Professor Robert Carpick, is in the area of nanoscale characterization of oxide materials using AFM contact, adhesion, and conductivity measurements. The researcher will use AFM to characterize the nanomechanical and electronic behavior of a range of oxide material interfaces as a function of contact cycles, applied bias voltage, and environment. Characterization of the composition, bonding, and structure of the oxides via TEM, XPS, and other methods will be extensively used, and TEM will be further used to determine changes in the oxides that occur after contact cycling experiments.

The successful applicant (recent PhD with or without prior postdoctoral study) should have extensive experience in using AFM to study nanomechanics/nanotribology and electronic behavior at the nanoscale. Experience with TEM is highly desirable, as is experience or familiarity with other material and surface characterization methods including XPS, SEM, analytical electron TEM or SEM methods (EDS, EELS), and focused ion beam milling. Experience studying the properties of metal oxide thin films and surfaces is desirable.

For both positions, the candidate should be fluent in spoken and written English, and be able to work independently and collaboratively. The candidate should be highly organized, motivated, and

driven. Based at the University of Pennsylvania (Philadelphia, USA), the Postdoctoral Fellow will work with collaborators at Carnegie Mellon University and in Hong Kong. We anticipate that both positions will last for at least 2 years (renewable annually). Both positions are available immediately.

Applicants should submit their applications by email to srol@seas.upenn.edu for the first position (DFT/MD), and to carpick@seas.upenn.edu for the second position (AFM). Include a cover letter that summarizes prior research fields and experience, and that addresses the qualifications for the position with respect to the descriptions above. Also include a CV with a list of published work, 2 representative publications, and the names and contact information of at least 2 references.

The University of Pennsylvania is an affirmative action/equal opportunity employer. All qualified applicants will receive consideration for employment and will not be discriminated against on the basis of race, color, religion, sex, sexual orientation, gender identity, creed, national or ethnic origin, citizenship status, disability, veteran status, or any other characteristic protected by law.

