

May 14, 2021

Postdoctoral Position at Washington University in St. Louis on the Atomistic Modeling of Chalcogenides

A one-year postdoctoral position with possible extension up to two years is available in the [Materials Modeling & Microscopy \(M-cube\) group](#) of [Rohan Mishra](#) at Washington University in St. Louis, beginning immediately. The successful candidate will use first-principles density-functional-theory (DFT) calculations along with group-theoretical methods for developing structure-property correlations in optically and electrically active chalcogenide perovskites.

Specifically, the work will focus on elucidating the effect of structural phase transitions in chalcogenide perovskites on their electrical polarization, optical properties and thermal properties. This project is a part of a multi-university effort and will involve extensive collaboration with experimentalists focused on the synthesis and characterization of these materials.

A second research thrust within our group involves atomic scale characterization of materials using aberration-corrected scanning transmission electron microscopy (STEM) and combining them with DFT calculations. The successful applicant is expected to be closely involved in this thrust and complement the microscopy work with DFT calculations and STEM image simulations to develop an understanding of the role of defects and interfaces on the functional properties of chalcogenide perovskites.

Applicants must have a recent Ph.D. in Materials Science, Physics, or a closely related field with demonstrated expertise in combining DFT calculations with group-theoretical tools to develop structure-property correlations in functional materials. The applicant should be able to work independently and in a team. Candidates with strong programming skills (using either Python, Fortran, or C/C++) will be preferred.

The successful applicant will have ample opportunities for career development. They are expected to be involved in co-mentoring graduate and undergraduate researchers, present their research at conferences, and develop independent research directions.

Interested candidates are encouraged to apply by emailing a single PDF file containing: (1) a cover letter (not more than one-page) with a summary of accomplishments and future research interests; (2) CV (with a list of all publications); and (3) names of at least two references to rmishra@wustl.edu.

Screening of applications will start immediately and will continue until the position is filled.