



Washington University in St. Louis

JAMES MCKELVEY SCHOOL OF ENGINEERING

Mechanical Engineering and Materials Science

June 10, 2022

Postdoctoral Position at Washington University in St. Louis on 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 for developing structure-property correlations in chalcogenide materials.

We are currently interested in quasi-one-dimensional (1D) chalcogenides for their optical and thermal properties, and 2D chalcogenide alloys for their electrocatalytic activity. The successful applicant is expected to develop quantitative structure-property-processing correlations to enable the design of new 1D and 2D chalcogenides for optical, thermal and electrocatalytic applications. These projects are part of multi-university collaborative efforts and involve extensive collaboration with experimentalists focused on the synthesis and characterization of these materials. The successful applicant is expected to work closely with our collaborators.

Applicants must have a recent Ph.D. in Materials Science, Physics, or a closely related field with demonstrated expertise in using DFT calculations to develop structure-property correlations in functional materials. Prior experience of developing phenomenological models from first-principles calculations will be a bonus. The applicant should be able to work independently and in a team. Candidates with strong programming skills (using 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 three references to rmishra@wustl.edu.

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