

March 6, 2024

Three Postdoctoral Openings at Washington University on First-principles-based Design of Materials

The **Materials Modeling & Microscopy (M-cube) group** of **Rohan Mishra** at Washington University in St. Louis is looking to fill **three postdoctoral openings, starting immediately**. These positions will be initially for 1 year, and renewable upon satisfactory progress for up to a total of three years.

Position 1 involves the screening of thermodynamically stable high-entropy alloys using first-principles density-functional theory (DFT) calculations, thermodynamic solution theory and machine-learning .

Position 2 involves first-principles-based investigation of point and extended defects, and chemical reactivity of sunlight-reflecting nanoparticles for use in stratospheric aerosol injection.

Position 3 involves first-principles-based design of multinary oxides, chalcogenides, and phosphides for use as electrocatalysts for oxygen evolution reaction.

All the projects are part of multi-PI and/or multi-university efforts and involve extensive collaboration with experimentalists focused on the synthesis and characterization of the targeted materials.

Applicants must have a recent Ph.D. in Materials Science, or a closely related field, with demonstrated expertise in using DFT calculations to develop structure-property correlations in materials. Candidates with prior experience in using machine-learning methods for screening materials and strong programming skills will be preferred. The applicants should be able to work independently and in a team.

Successful applicants 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.

Washington University in St. Louis is a private university with about 16,000 students. It is surrounded by and adjacent to museums, performance venues, vibrant entertainment and dining districts, one of the nation's largest civic parks, and beautiful, tree-lined neighborhoods rich in history and diversity. [St. Louis](#) is consistently ranked among the nation's most affordable and best places to live.

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. Candidates should also mention the position(s) they are interested in.
2. CV with a list of all publications
3. Names of three references.

The email should be sent to Prof. Mishra (rmishra@wustl.edu). Please use "Spring 2024 postdoc openings" in the subject line. Screening of applications will start immediately and will continue until the positions are filled.