Mechanical Engineering and Materials Science

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Postdoctoral Position at Washington University in St. Louis on Modeling of Perovskite Semiconductors

A one-year postdoctoral position with possible extension up to two years is available in the Materials Modeling & Microscopy 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 materials and nanostructures.

Specifically, the work will focus on elucidating the role of defects, surfaces and interfaces in halide, chalcogenide and oxide perovskites for various applications including in solar cells, light-emitting diodes, and as single-photon emitters. The project will involve extensive collaboration with experimentalists focused on synthesis and characterization of the 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 atomic-scale structure-property correlations.

Applicants must have a recent Ph.D. in Materials Science, Physics, or a closely related field with expertise in applying DFT to develop structure-property correlations in materials. The applicant should be able to work independently and in a team involving experimental collaborators. Candidates with strong programing skills (using either Python, Fortran, or C/C++) will be preferred.

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.