

MIT Job Description

Post-Doctoral Research Associate: MIT, Department of Chemical Engineering, Group of Bernhardt Trout

Position: Computational Viral Assembly

Position Overview:

A full-time postdoctoral research associate position is open in the Molecular Engineering Laboratory (Trout Research Group) in the Department of Chemical Engineering at MIT to investigate the reaction mechanisms of cysteine-cysteine bond formation using computational *ab initio* methods. Specifically, we are working with a major pharmaceutical company to understand the role of oxidants and transition metals in S-S bond formation during viral assembly. As a postdoc, this person will perform high-level *ab initio* studies to determine the energetics of reaction pathways with various different transition metal catalysts and solvent environments. The postdoc will develop a rational understanding of these reactions and propose optimal conditions to be validated through experiment. The position requires strong collaboration with experimentalists and the pharmaceutical industry, and requires regular research progress reports to pharmaceutical scientists and managers, in addition to visiting the company.

Minimum Qualifications:

PhD in Theoretical and Computational Chemistry, Chemical Engineering, Physics, or related field. Must be a skilled professional with expertise in *ab initio* methods, QM/MM models, molecular dynamics, and mathematical modeling.

Preferred Qualifications:

Demonstrated experience in a wide range of theoretical and computational chemistry methodologies as well as a proven publication track record. Preference for experience with *ab initio* computations of transition metals. Ideally, experience with molecular dynamics and/or QM/MM computations. Proven ability to work independently as well as experience in managing several projects simultaneously. Strong programming skills.

In addition to applying online to the above job ID, please send CV and cover letter including the names of two references to Michael Bellucci (bellucci@mit.edu) with "Viral Assembly Post-Doc" in the subject line.