

## **Postdoctoral Associate--Chemistry and Chemical Biology (Ithaca, NY)**

This postdoctoral position involves primary research and related professional activities associated with the application and development of new algorithms for understanding allostery, protein conformational change, and drug development. Will conduct research on new computational approaches integrating machine learning with biomolecular simulation to better understand proteins and find new drug candidates.

### **DUTIES AND RESPONSIBILITIES:**

Engage in innovative research related to the integration of machine learning, biomolecular simulation, and experimental data to get new insights into the basic science of proteins and the development of new drugs to address pressing disease challenges. The positions will require becoming proficient in performing molecular dynamics simulations, designing, and applying innovative machine learning algorithms, and interfacing with experimental data. Particular areas of focus include the development of new drug candidates to target tuberculosis, as well as integration of experimental structural biology techniques with molecular simulation.

The associate will draft and submit multiple manuscripts for publication in top-level peer-reviewed scientific journals; present results at professional meetings, conferences, and popular seminars. Assist in training of undergraduate lab assistants and undergraduates carrying out research projects, and new or rotating graduate students. The candidate is also expected to engage in ongoing academic and intellectual life within relevant scientific programs in the Department of Chemistry and Chemical Biology and collaborate with groups members in the research laboratory.

*This is a 12-month Academic appointment, which is renewable depending on funding and performance.*

**QUALIFICATIONS:** Ph.D. in chemistry or related fields with coding ability. Background in related areas of research. These include, but are not limited to:

- Molecular Simulation, particularly advanced algorithms such as enhanced sampling, Markov state modeling and related algorithms, and coarse-grained simulation.
- Machine Learning, particularly geometric ML, equivariant ML, transformers, and generative models.
- Computational Statistics, particularly high-dimensional data and MCMC.
- Experimental structural biology techniques particularly Cryo-EM and Cryo-ET.
- The biology of *Mycobacterium tuberculosis*, particularly its structural biology and biochemistry.

**PAY RANGE:** \$56,484 - \$75,000

**START:** August 2023 at earliest.

Interested candidates should submit a cover letter and Curriculum Vitae to Dr. Erik Thiede at eht45 [at] cornell.edu with your curriculum vitae and the favorite research paper that you have written.