Postdoctoral Fellow – Computational Molecular Modeling

Position Summary:
Tougaloo College is seeking a highly motivated Postdoctoral Fellow to join our team as part of the Mississippi Nano-Bio ImmunoEngineering Consortium (NIEC), a statewide, NSF-funded, multidisciplinary research network focused on advancing next-generation biomaterials, nanomedicine, and immunoengineering. The preferred start date is October 1, 2025, with an appointment for 1–2 years, and a possible extension contingent upon funding availability. For questions, contact: kkapusta@tougaloo.edu.

Essential Responsibilities:
The successful candidate will contribute to cutting-edge research using computational modeling approaches, working in close collaboration with chemists, biologists, and chemical engineers. Responsibilities include conducting advanced computational simulations aligned with NIEC's research priorities, including molecular docking, molecular dynamics, free energy perturbation (FEP), (Q)SAR, and machine learning-based studies. The postdoctoral fellow will apply and refine state-of-the-art computational methods to model complex biomolecular systems; prepare peer-reviewed publications; present research at local, regional, and national conferences; and mentor undergraduate researchers in computational chemistry and biology. Additional responsibilities include assisting with laboratory operations, maintaining software environments, ensuring data management best practices, and engaging in interdisciplinary collaborations across NIEC partner institutions.

Required Experience/Knowledge/Skills:
• Ph.D. in Computational Chemistry, Physics, Biology, or Chemical Engineering, or a closely related field from an accredited institution.
• Demonstrated experience in computational modeling and molecular simulation techniques.
• Proficiency in relevant tools such as molecular docking, MD simulations, FEP, or QSAR methods.
• Working knowledge of computational chemistry and biochemistry principles. • Strong written and verbal communication skills.
• Ability to work independently and as part of a collaborative, multidisciplinary research team.

Preferred Qualifications:
• Experience working with high-performance computing (HPC) systems and system software administration.
• Familiarity with Python or R programming.
• Experience in chemical/biological/bioinformatics data analysis, especially large-scale or multi-omics datasets.
• Exposure to modern ML/AI algorithms for molecular modeling or drug discovery.
• Proficiency with Schrödinger Suite, MOE, NAMD, or similar computational chemistry software packages.

Application Instructions:
Applications will be reviewed immediately and continue until the position is filled. Applicants must submit a cover letter, a current curriculum vitae, and three letters of recommendation. Applicants must be eligible to work in the U.S. or qualify for a J-1 visa. Unfortunately, H-1B visa sponsorship is unavailable for this position due to funding limitations.

Date of Position Opening:	**08/11/2025**
Application Deadline:	**Until position filled**
Salary:	**$40,000 annually**
Job Listings:	**https://www.tougaloo.edu/about-tougaloo-college/jobs**
**Email App/Resume/Cover Letter to:	**TougalooCareers@tougaloo.edu**
Physical Address:	**Tougaloo College**
	Attention: Director of Human Resources
	500 West County Line Road
	Tougaloo, MS 39174