We have an opening for one postdoctoral researcher to work at the University of Maryland, College Park in joint collaboration with the groups of Pratyush Tiwary and John Weeks, for a DOE-BES funded project titled “Modeling liquids, interfaces and nucleation with Local Molecular Field theory and Artificial Intelligence sampling methods”.

Scope of the work: Together with Weeks, Tiwary and graduate/undergraduate students, you will develop and apply new theoretical and computational tools for the study of thermodynamics and kinetics of nucleation and solvation in nonuniform polar liquids, focusing on processes occurring at solid-liquid and liquid-vapor interfaces. These tools will combine insights from Local Molecular Field (LMF) theory for systems with strong Coulomb interactions [Gao, Remsing, Weeks, Proc. Natl. Acad. Sci. 117 1293 (2020)] with those from advanced sampling methods such as metadynamics [Tiwary, Parrinello, Phys. Rev. Lett. 111 230602 (2013)] and more recent Artificial Intelligence (AI) based sampling methods [Wang, Ribeiro, Tiwary, Nature Commun. 10 3573 (2019)]. The combined approach should provide both new physical insights into the complex physics occurring in the liquid, solid or vapor phases, and also permit even more efficient sampling simulations. We will first study crystal nucleation of molecular systems such as urea and calcium carbonate where naive use of classical nucleation theory has been found unsatisfactory. We will also develop a general AI based framework that we believe can uncover some of the physically based insights and reduced representations used in LMF and related theories, and possibly reveal new currently unappreciated insights. More generally, we hope to develop appropriately modified AI algorithms that work in conjunction with intuitive general physical ideas, each suggesting qualitatively new directions, with AI carrying out most of the detailed quantitative connections and extensions on its own.

You can read further publications from the Weeks and Tiwary groups here:
https://scholar.google.com/citations?user=2w06tQsAAAAJ
https://scholar.google.com/citations?user=v-NQD2cAAAAJ

What we are looking for: The candidate should have a PhD degree in physics, chemistry, chemical physics, materials science, or a related field. The candidate should have demonstrated experience in statistical mechanics and molecular simulations, and fluency in at least one programming language. Including your GitHub page link in your resume would be very useful. Experience with machine learning platforms is desired but not mandatory.

Further details: The appointment can start on September 1, 2020 or at a later time on mutual agreement. The initial appointment is for a period of one year and the contract is renewable for another year, pending satisfactory research progress and availability of research funds. Applicants from all nationalities are welcome - international applicants will however need to make sure to meet various requirements for procuring appropriate visas. Review of applications will begin immediately and continue until the position is filled.

Please email your resume to ptiwary at umd dot edu, along with a brief cover letter stating your research interests and aspirations. Please make sure to include contact information for at least three references.

The Tiwary and Weeks research groups at the University of Maryland are located in the Department of Chemistry and Biochemistry, and the Institute for Physical Science & Technology, less than 10 miles from Washington D.C. The University of Maryland is an Equal Employment/ Affirmative Action employer. We do not discriminate in hiring on the basis of sex, gender identity, sexual orientation, race, color, religious creed, national origin, physical or mental disability, protected Veteran status, or any other characteristic protected by federal, state, or local law.