Joint OpenFF-XtalPi Distinguished Postdoctoral Fellowship

The Open Force Field Consortium (OpenFF, openforcefield.org) and XtalPi, Inc. (xtalpi.com) seeks a Distinguished Postdoctoral Fellow to perform cutting-edge research in a unique academic-industrial joint effort.

OpenFF is an academic collaboration (based at UC Irvine / UC Davis / UC San Diego / Univ. Colorado Boulder / Sloan Kettering Institute in New York) that seeks to develop next-generation molecular mechanics force fields and associated parameterization software and data infrastructure. XtalPi is a pharmaceutical technology company founded in 2014 that is introducing revolutionary advances in drug research and development, and has established strategic partnerships with several major pharmaceutical companies and recently completed a Series B funding round with Sequoia, Tencent, and Google.

The Postdoctoral Fellow will work with OpenFF and XtalPi to improve the accuracy of molecular mechanics force fields for predicting crystal structures and binding free energies. The work spans the disciplines of force field development/validation and Bayesian inference, and seeks to answer the fundamental scientific questions: 1) What regions of chemical space are critical failures for current force fields? 2) What are the fundamental limitations of (a) current functional forms and (b) parameterization methods?

The position spans a two-year project period that involves a gradual transition from the OpenFF side to the XtalPi side. In Year 1, the Fellow will be hosted for ~9 months in one of the academic groups (to be determined by the OpenFF PIs, XtalPi, and the Fellow) and ~3 months at XtalPi in Shenzhen, China or Boston, MA. In Year 2, the time division will be 3-6 months academic / 6-9 months XtalPi. The Fellow will be considered for full-time employment at XtalPi after Year 2.

We seek a highly talented candidate for this position with the following skills:

- A Ph.D. in physics, chemistry, chemical engineering or a related field is required;
- Significant experience with molecular simulations is desired;
- Solid background in statistical mechanics and programming is desired;
- Good understanding of force field formats and software representations is desired;
- Good cheminformatics experience/understanding is desired;
- Good understanding of space groups for crystal structure operations is desired;
- Experience with machine learning and/or Bayesian inference is desired.

The position includes a competitive salary and benefits, as well as housing arrangements to defray the costs of living and working in two geographical locations. To apply, send a cover letter including a description of research interests, CV or resume, and contact information for at least three references including name, institution, and email address to leeping (at) ucdavis.edu and/or szhr (at) xtalpi.com to be distributed to OpenFF PIs and XtalPi scientists.

Applications should be received by June 1, 2018. The start date is planned for Fall 2018.