Title TBD

In 1953 Stanley Miller mixed methane, ammonia, and hydrogen in glass tubes. A flask with heated water and one with electrodes connected the tubes, and when a spark of electricity bolted across the electrodes, the apparatus produced amino acids, the building blocks of all proteins. When I first heard about this experiment in high school, I was attracted to its simplicity and elegance. Now, I recognize that it’s explanatory power originates in the novelty of looking at a seemingly impenetrable question—the origin of life—from a new perspective. I’m interested in research environments where disciplines are combined to tackle problems on the boundary of biological and medical science.

The central theme of my research is uncovering the physical principles that underlie biological and chemical phenomena.

# Summary of previous research

## Improving free energy calculations

Accurate binding thermodynamics calculations remain one of the central goals of biomolecular simulations. While in the Gilson group, I contributed to an overall evaluation of more than ten different methods, from research groups around the world, used to compute host-guest binding free energies and enthalpies[1](#ref-BGsUYQln). As part of that work, I extended our own method (attach-pull-release[2](#ref-uzHaEv9Z)) by completely rewriting the code in Python and adding several advanced features enabling larger and more challenging systems to be used (this code is available on [GitHub](https://www.github.com/slochower/pAPRika)). More recently, I have also worked on assessing the efficiency and reproducibility of how different algorithms converge toward free energy estimates (forthcoming publication).

## The evolution of molecular motors

Biological motors are enzymes that use chemical energy to drive directional motion. Although motor proteins must have arisen through random mutation and natural selection, it is not clear how the evolutionary leap from non-motor enzymes to molecular motors could have occurred. I showed that any chiral molecule driven out of equilibrium should undergo cycles of conformational change[3](#ref-1BfYw0gk2). This work was highlighted by [UCSD](http://ucsdhealthsciences.tumblr.com/post/173707350285/its-not-intelligent-design-so-how-did) and [“New and Notable”](https://www.cell.com/biophysj/fulltext/S0006-3495(18)30444-2) in Biophysical Journal.

## The design of new force fields

As part of the open force field consortium—a collaboration with Dr. David Mobley, Dr. John Chodera, Dr. Michael Shirts, Dr. Lee-Ping Wang, and Dr. Chris Bayly— I have participated in the effort to build new molecular mechanics force fields based on direct chemical perception (forthcoming publication) instead of indirect, atom-type based approaches. I have also contributed to the design, coding, and implementation of a new force field format—SMIRKS Native Open Force Field (SMIRNOFF)—based on a hierarchical structure that supports customized combining rules, partial bond orders, polarizability, and other advanced features. The tools and data are open source and available on [GitHub](https://github.com/openforcefield).

## Simulations of complex membranes

Continuing the work that I started during graduate school at the University of Pennsylvania[4](#ref-1G0A01ZNq)–[8](#ref-1AHXI1BtY), I’m interested in simulating increasingly complex, and thus more physiologically relevant, models of biological membranes. We recently reported (forthcoming publication) how the interplay between lipid species, cholesterol, counterions, and water near the membrane interface can lead to the formation of nano-scale lipid clusters. A natural next step is to understand the role proteins play in stabilizing these clusters, as discussed below.