William A. Brookshire
Department of Chemical
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ChBE Seminar Series

Learning How to Build Molecules that Fold Like Proteins

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Nature carries out an astonishing variety of biological functions with a very limited set of chemical building blocks. Biological heteropolymers can achieve highly specific functions because of their well-defined three-dimensional arrangements. This three-dimensional structure is controlled by the chemistry of the monomer backbone and interactions of involving specified sequences of side chains. The expansive range of function achieved with a small set of chemical building blocks implies that there is a much larger range of materials that could be built with human-engineered heteropolymers that draw from a wider palette of chemical functionality. If we better understand how to predict the structures of nonbiological heteropolymers and modulate their relative stability, we can make materials that are more chemically resilient, more responsive, and mechanically tougher, and that act as more adaptable smart materials, more efficient catalysts, and better electron conductors.

In this talk I describe work in our group so far to start from basic physical principles and interactions to build molecularly inspired simple models that can capture the physics of oligomers that cooperatively fold into defined secondary structures in similar ways to proteins. I describe our modeling philosophy to achieve this, and show the sorts of cooperative folding behavior that can be captured with even the simplest of models. What more might need to be done to understand how to build true non-protein molecular machines?

Michael Shirts is a Professor of Chemical and Biological Engineering at the University of Colorado Boulder. He works on computational soft matter problems ranging from drug design to membrane separations, with a special emphasis in developing tools to make molecular simulation more robust, predictive, and reliable. He was an undergraduate at Harvard and received a PhD from Stanford, where he was a Fannie and John Hertz Fellow and helped start Folding@Home, the distributed science project for protein biophysics. He also helped found the Open Force Field Initiative, an open science, industry-academic joint effort to design better tools for force field parameterization, and is a founder and managing editor of the open-access Living Journal of Computational Molecular Science. He has received awards including the NSF CAREER and the AIChE CoMSEF Impact award.

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