CHEMICAL ENGINEERING

SEMINAR SERIES

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Why can't we engineer drugs on a computer? And what can be done about it?

ABSTRACT: The design of airplanes, bridges, chemical plants, and computer chips is aided significantly by modern computational tools. Design of novel molecular entities, however, is done primarily by trial-and-error. A prime example is the pharmaceutical industry, where the complexity of biomolecular interactions has greatly limited our ability to model and design effective small molecule drugs. This means drug design has remained somewhat of a black art, relying on many ad hoc assumptions and on the intuitive insights of experienced medicinal chemists.

What are the barriers that must be overcome in order to model drug-ligand binding affinities, solubilities, partitioning into delivery formulations and polymorph stabilities effectively? Is there a hope to change the process of designing drugs with high affinities and a specific mode of action from a trial-and-error art to a nanoscale engineering process using high-quality, reliable modeling?

I will discuss research in our group working towards the goal of modeling noncovalent interactions sufficiently reliable and efficient to have a place in the pharmaceutical workflow.

RECEPTION 3:30   •   LECTURE 4:00 - 5:00
PHYSICS ASTRONOMY BLDG. (PAA)   A110

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BIOGRAPHY: Dr. Shirts is an associate professor of Chemical and Biological Engineering at the University of Colorado Boulder. He received his A.B. in chemistry from Harvard and his Ph.D. in Chemistry from Stanford, where he was a Hertz Fellow. At Stanford, he helped found the Folding@Home distributed computing platform, which allows hundreds of thousands of volunteers to contribute their spare CPU cycles to solve biophysical problems, and was afterwards an NIH NRSA Fellow at Columbia University. He is a developer of the GROMACS molecular simulation program, and has been awarded an ACS Computers in Chemistry Young Investigator award and an NSF CAREER award.