Jeffrey Saven: Group expertise: theoretical chemistry, molecular modeling, simulation and design. The group has an extensive record of the molecular simulation of proteins, polymers and other macromolecules in solvated environments. The group has developed methods for designing proteins and addressing their sequence and chemical variability. These methods have been applied extensively to design new proteins de novo and to redesign existing proteins. In addition to the development and application of theoretical and computational methods, the group experimentally synthesizes, expresses and characterizes designed proteins. Major efforts include (a) design of proteins that bind selectively and with high affinity to specific ligands and cofactors, such as electro-optically active porphryn-based cofactors, (b) redesign of natural proteins, including membrane proteins (ion channels and receptors) to better understand and engineer these systems, and (c) design of proteins to interact with nonbiological nanostructures, and (d) simulations of polymers interacting with carbon nanostructures. ** saven@sas.upenn.edu