CBST Seminar

Center for Biomanufacturing Science & Technology

UNIVERSITY OF DELAWARE

Dr. Jeffrey Gray

Professor, Chemical and Biomolecular Engineering

Johns Hopkins University

DATE:
March 23, 2016
TIME:
2:00 p.m.
LOCATION:
366 Colburn Lab

Professor Gray received his B.S.E. in chemical engineering at the University of Michigan and his Ph.D. in chemical engineering at the University of Texas at Austin. He completed post-doctoral training researching protein-protein docking at the University of Washington. In 2002 he joined Johns Hopkins University as an Assistant Professor and in 2009 he was promoted to Associate Professor with Tenure. In the Spring of 2013 he was a Visiting Professor at the University of Texas at Austin, and in 2014 he was promoted to Professor.

His research focuses on computational protein structure prediction and design, particularly protein-protein docking, therapeutic antibodies, and protein-surface interactions. Gray's lab leads the development of RosettaDock, RosettaAntibody, the ROSIE web server, and the PyRosetta interactive platform for protein structure prediction and design; these tools are used widely by the research community. Gray's lab has produced the most accurate complex structure for several targets in the CAPRI blind protein-protein docking challenge and sub-angstrom antibody binding loop structures in the Antibody Modeling Assessment. Gray's work has been funded by NIH, NSF, DARPA, ACS, the Beckman Foundation, and the UCB pharmaceutical company. As of March 2016, he has authored over 72 papers which have attracted over 4,200 citations. He has supervised 10 post-docs, 20 graduate students, 45 undergraduate students, and several high school students.

Gray has received the Beckman Young Investigator Award, the Johns Hopkins Alumni Association Excellence in Teaching Award, and the National Science Foundation's CAREER Award, and he was named the F. Stuart Hodgson Faculty Scholar. In 2016 he was elected to the College of Fellows of the American Institute of Medical and Biological Engineering (AIMBE). He serves on the editorial board of Proteins, on the scientific advisory board of the Rosetta Design Group, and from 2005-2015 he served on the board of directors of the Ingenuity Project. He is a champion of broadening participation in science and engineering, serving as a member of the Johns Hopkins Diversity Leadership Council and as the Diversity Chair of the Rosetta Commons. He is also the Director of the NSF-supported Rosetta Commons Summer Intern Program.

"Computational Protein Engineering of Crystal Growth, Membrane Proteins, and Glycoproteins"

Biomanufacturing products depend on the interactions between biomolecules, and these interactions in turn arise from the molecular sequences and structures. Computational protein engineering methods offer potential to predict and design behaviors from protein solubility to enzymatic activity. My lab has develops computational tools to study the atomic structure of protein interfaces to explain not only how biological and disease processes work but also how one might go about altering these processes at the molecular level. Creating computational tools first requires solving problems of basic science including (1) how to sample the myriad conformations available to proteins and (2) how to accurately calculate the energy of each conformation. In this talk, I will relay three stories. First, I will present the de novo design of peptides that can control mineral growth through our efforts to guide the growth of calcite. Second, I will describe a general framework for membrane protein modeling and design that combines scoring, conformational sampling, and mutation routines for refinement, mutagenesis, docking, and symmetric assembly. Finally, I will present new tools for modeling the three-dimensional structures of oligosaccharides, polysaccharides, and glycoproteins by sampling ring, backbone, and side chain conformations for applications in enzymology, immunology, and crystallography.