

PHYSICS COLLOQUIUM, partially funded by the GSFEI

David Baker
UW Biochemistry

“Prediction and design of macromolecular structures and interactions”

Monday, 11/6

4:00 P.M., Ronald Geballe Auditorium, A-102, PAA

Reception at 3:45 P.M. in the lobby

seminars



November 06-09, 2006

Abstract: I will discuss efforts towards transforming structural biology from a largely experimental science to a primarily computational science. Specifically, I will describe:

(1) Significant progress in ab initio computation of the structures of small proteins from sequence information alone. Using over 100,000 computers distributed around the world, and a physically realistic atomic level forcefield, we can predict structures to less than 2-3Å from the crystal structure for a number of small proteins (Bradley et al, Science 2005; boinc.bakerlab.org/rosetta/top_predictions.html). (2) The high accuracy prediction of structures of protein-protein complexes from the structures of the isolated proteins for cases where there are not significant conformational changes, and our progress in docking with backbone flexibility (Furman et al, Science 2005). (3) The computer based design of novel highly specific endonucleases for targeted genomics applications such as gene therapy (Ashworth et al, Nature 441(7093):656-9). (4) The design of new protein folds and protein interactions, and ongoing efforts to computationally design catalysts for reactions not catalyzed by naturally occurring enzymes and a vaccine for HIV.

Monday, 11/6

INT Seminar Alejandro Ayala, Instituto de Ciencias Nucleares
10:00 A.M., Rm. C-421, PAT “Proton to Pion Ratio at RHIC”

Tuesday, 11/7

INT Seminar Kevin Dusling, SUNY Stony Brook
10:00 A.M., Rm. C-421, PAT “Molecular Dynamic Simulation of Color Diffusion and Parton Energy Loss in a Classical sQGP”

Particle Theory Seminar Veronica Sanz, Boston University
2:30 A.M., Rm. C-421, PAT “The fifth dimension as an analogue computer of strong interactions at the LHC”

Condensed Matter Seminar Raghu Parthasarathy, University of Oregon
4:00 P.M., Rm. C-421, PAT “Spatial organization of, at, and by lipid membranes”

Wednesday, 11/8

INT Seminar Javier Lopez Albacete, Ohio State University
10:00 A.M., Rm. C-421, PAT “Heavy Quark Production in pA Collisions”

Thursday, 11/9

INT Seminar Ian Balitsky, Old Dominion University
10:00 A.M., Rm. C-421, PAT “Quark Contribution to the Small-x Evolution of a Color Dipole”

Astronomy Colloquium Roger Romani, Stanford
4:00 P.M., Rm. A-102, PAA “Putting ‘English’ on a Neutron Star”

Friday, 11/10

INT Seminar Shunzo Kumano, KEK
10:00 A.M., Rm. C-421, PAT “Recent Progress on the Determination of Nuclear Parton Distribution Functions”

Particle Astrophysics Seminar Eric Thrane, UW Physics
3:30 P.M., Rm. A-110, PAA “Q-Balls in Super-K”