THE
CATHOLIC UNIVERSITY
of AMERICA

Department of Physics
Colloquium

Dr. Peter J. Steinbach
National Institute of Health
Center of Molecular Modeling

Modeling Protein Energy Landscapes

Newtonian descriptions of atomic interactions have been a cornerstone of computational structural biology for decades, from the refinement of macromolecular structures obtained using x-ray diffraction or nuclear magnetic resonance to the prediction of structures and the simulation of dynamics. After a brief introduction to protein structure and classical simulation, the modeling of the human cannabinoid-1 receptor, a target in the design of drugs for obesity and diabetes, will be discussed. Subsequently confirmed by x-ray crystallography, this model was used successfully to guide mutagenesis experiments. Then, recent progress in *ab initio* prediction of protein structure, using a simplified and refined continuum solvent model based on screened Coulomb potentials, will be presented.

Wednesday, December 6, 2017
4:00pm
108 Hannan Hall
Refreshments will be served at 3:45

Sponsored in part by the Graduate Student Association
For more information or if you would like to request disability accommodations, please contact:
Patrick Burke **(202) 319-5315**