Science at the Edge Seminar Series

Quantitative Biology/Gene Expression in Development and Disease
Joint with Department of Mathematics

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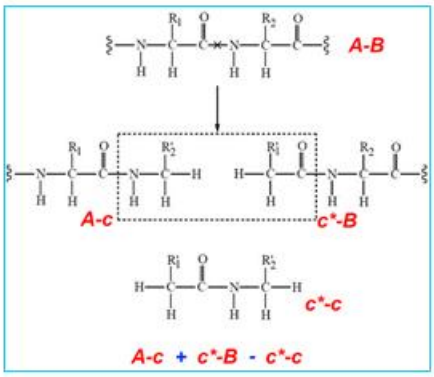
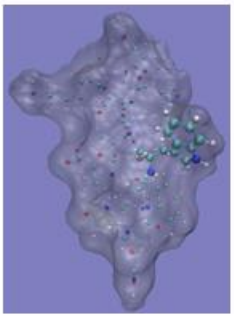
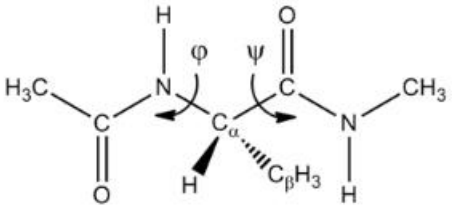
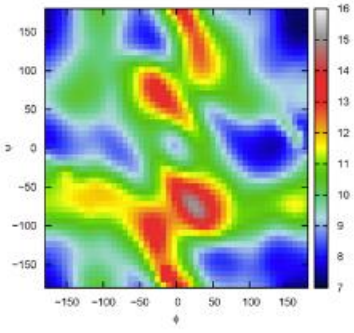
Towards a New Force Field

The widely used conventional force fields suffer from lack of explicit polarization effect and limited accuracy in reproducing the distribution of main chain dihedrals. In the past few years, we have been devoted to calibrating AMBER force fields by employing polarization effect and introducing new main chain torsion energy terms. I will start this talk with a molecular tailoring method termed the Molecular Fractionation with Conjugate Caps, which was developed by Prof. John ZH Zhang ten years ago in NYU. With this method, calculation of the whole protein at quantum mechanical level is feasible and polarized protein-specific charge can be obtained from the distorted electronic structure of the protein fragments. Some applications of this charge model will be presented. I will also introduce our recent progress in the implementation and parameterization of a coupled main torsion energy term, which has been shown to be quite successful in reproducing the J coupling data for short peptides and in protein folding simulations.









$$E(\phi,\psi) = \sum_{m=-N_\phi}^{N_\phi} \sum_{n=-N_\psi}^{N_\psi} C(m,n) e^{-im\phi} e^{-in\psi}$$

Monday, April 7, 2014 at 10:30 a.m.
Room 1400 BPS
Refreshments at 10:15