Protein Folding and Unfolding by Quantum Mechanics

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Abstract

Proteins are sensitive to electrostatic charges from amino acid side chains that change with conformation. But MD simulations of protein folding and unfolding are based on classical force fields with electrostatic interaction [1-3] represented by fixed point charges. MD stands for molecular dynamics. QM modification of point charges during conformational changes is required, but is impractical because of computational costs. QM stands for quantum mechanics.

Computation costs aside, even if point charges were continuously updated, the effect on protein folding and unfolding would be insignificant compared to the more fundamental QM effect of the Planck law on the heat capacity of atoms. In this regard, proteins are generally thought to unfold upon increasing temperature based on the classical assumption the constituent atoms have heat capacity. But the Planck law requires the heat capacity of the atom to vanish with conservation [4] proceeding by creating EM radiation that by the photoelectric effect removes electrons to positively charge the protein atoms. What this means is the heat thought to induce unfolding by increasing the temperature of proteins is actually conserved by producing charge that unfolds the protein by Coulomb repulsion.

To illustrate QM induced charge, the MD simulation of folding and unfolding using [5] for a simple 5-atom protein is illustrated in Figure 1. Initially, the protein in the form of a semi-circle relaxes under L-J forces, but does not unfold. L-J stands for Lennard-Jones. Unfolding occurs upon applying QM induced repulsive positive charge (0.5 – 1 electron charges) on each atom. Folding back to an intermediate cluster occurs by relaxing the protein with L-J forces alone without QM induced charge. The protein returns to an inverted semi-circular shape by unfolding the cluster by applying the QM induced repulsive charge. How the protein constantly modifies QM induced charge is discussed.

Image

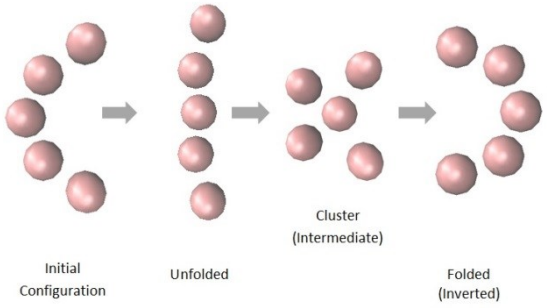

Figure 1: QM induced charge in Protein folding and unfolding

Recent Publications

1. Changge Ji, Ye Mei (2014) Some Practical Approaches to Treating Electrostatic Polarization of Proteins. Accounts of Chemical Research ACS dx.doi.org/10.1021/ar500094n.
2. Weber JK, Pande VS (2012) Protein Folding Is Mechanistically Robust. Biophysical Journal 102: 859–867.
3. Torshin IY, Harrison RW (2003) Protein Folding: Search for Basic Physical Models. The Scientific World JOURNAL 623–635.
4. Prevenslik TV (2010-2018) Simple QED Applications at the nanoscale. See http://www.nanoqed.org
5. Allen MP, Tildesley, DJ (1987) *Computer Simulation of Liquids*, Oxford University Press.

Biography

Thomas Prevenslik developed the simple theory of QED based on the Planck law of QM. Differing from the complex QED by Feynman and others, simple QED assumes any heat absorbed at the nanoscale having high surface-to-volume ratios place interior atoms under high EM confinement that by the Planck law of QM precludes the atoms from having the heat capacity to conserve heat by an increase in temperature. In the instant topic of *Protein Folding and Unfolding by Quantum Mechanics*, the atoms may only conserve heat by creating EM radiation that by removing electrons by the photoelectric effect charges the atoms positive inducing Coulomb repulsion that enhances unfolding. On a pico-second time scale, the electrons recombine with charged atoms to place the protein under van der Waals attraction that fold the protein. Driven by heat, protein folding and unfolding is the consequence of fluctuations between QM induced charge and neutral states.

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Notes/Comments: