Abstract Title: Protein Folding by Quantum Mechanics

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Abstract

Despite explaining protein folding using classical statistical mechanics and thermodynamics, few molecular dynamics (MD) simulations explicitly include basic physical electrostatics and Van der Waals forces. Although folding occurs with the protein in isolation, MD simulations are performed with periodic boundaries. Heat provides the denaturant, and is simulated by specifying the protein temperature. Classical thermodynamics assumes the native folded state of proteins to correspond lowest-energy states, but this is not always true. Moreover, folding is a rapid process that occurs on microsecond time scales, but the response of proteins having a hydrophobic interior is a slow process. In contrast, electrostatic effects propagating at light speed and are important for rapid kinetics, but neglected in MD simulations.

More fundamentally, current MD simulations are problematic because of the differences between classical physics and QM with respect to the heat capacity of the atom. QM stands for quantum mechanics. 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 of QM requires the heat capacity of the atom to vanish with conservation proceeding by creating EM radiation that 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 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 only 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. Upon applying the QM induced repulsive charge, the protein unfolds to an inverted semi-circular shape.

Keywords—*Protein folding, classical physics, quantum mechanics, molecular dynamics*

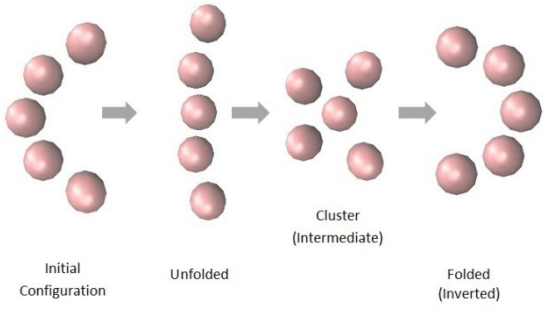

Figure 1 Protein Folding Simulation

Professional Biography

Thomas Prevenslik developed the simple theory of QED based on the Planck law of QM. 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 by Quantum Mechanics*, the protein atoms may only conserve heat by creating EM radiation that charges the atoms positive by removing electrons to the surrounding water, the Coulomb repulsion between atoms enhancing unfolding. On a pico-second time scale, the electrons attached to the water molecules recombine with charged protein atoms leaving only van der Waals attractive forces to induce folding. Driven by heat, subsequent protein folding and unfolding is the consequence of fluctuations between QM induced charged atoms and neutralization by electron–rich surrounding water molecules.

Recent Publications

- Changge J, Ye M (2014) Some Practical Approaches to Treating Electrostatic Polarization of Proteins. ACS Accounts of Chemical Research 136-140.
- Torshin IY, Harrison RW (2003) Protein Folding: Search for Basic Physical Models. The Scientific World Journal: 3, 623-63.
- Prevenslik TV (2010-2019) Simple QED Applications at the Nanoscale. See http://www.nanoqed.org

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Any Comments: