Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Analysis of Cavity Volumes in Proteins Using Percolation Theory

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Molecular packing is studied in a diverse set of globular proteins in their native state ranging in size from 34 to 839 residues An new algorithm has been developed that builds upon the classic Hoshen-Kopelman algorithm for site percolation combined with a local connection criterion that classifies empty space within a protein as a cavity when large enough to hold a spherical shaped probe of radius, R, otherwise a microvoid. Although microvoid cannot fit an object (e.g. molecule or ion) that is the size of the probe or larger, total microvoid volume is a major contribution to protein volume. Importantly, the cavity and microvoid classification depends on probe radius. As probe size decreases, less microvoid forms in favor of more cavities. As probe size is varied from large to small, many disconnected cavities merge to form a percolating path. For fixed probe size, microvoid, cavity and solvent accessible boundary volume properties reflect conformational fluctuations. These results are visualized on three-dimensional structures. Analysis of the cluster statistics within the framework of percolation theory suggests interconversion between microvoid and cavity pathways regulate the dynamics of solvent penetration during partial unfolding events important to protein function.

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Date submitted: 04 Nov 2015 Electronic form version 1.4