

E0052

The Role of Water in the Thermodynamics and Kinetics of Protein Crystallization. Peter G. Vekilov, Dept. of Chemical Engineering, Univ. of Houston, Houston, TX, 77204, vekilov@uh.edu.

Recent evidence shows that water, the native solvent of proteins, is structured at the hydrophobic and hydrophilic patches on the surface of the protein molecules. Examples will be provided illustrating that this structuring often determines the entropy and enthalpy balance of crystallization, leads to unusual intermolecular interaction potentials with one or more outlying maxima, which severely affect the phase diagrams, and that the dynamics of destruction of the water shell is the major determinant of the kinetics of association of molecules into crystals. Because of the water structuring, the fastest pathway of crystal nucleation is not the one with the lowest free-energy barriers.