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Glassy protein dynamics and gigantic solvent reorganization energy of plastocyanin DAVID LEBARD, DMITRY MATYUSHOV, Center for Biological Physics, Arizona State University — This work focuses on the results of extensive explicit solvent Molecular Dynamics simulations of plastocyanin, a blue copper electron transfer protein involved in natural photosynthesis. Simulation data indicate that low-frequency non-ergodic fluctuations of the protein matrix tethered to the hydrating water are responsible for a very broad distribution of the vertical energy gaps of one-electron protein reduction/oxidation. The width of the corresponding free energy surfaces yields a reorganization free energy far larger than previously reported for any organic, inorganic, or biological chromophores. However, the Stokes shift is not affected by these slow motions and can be calculated from the polarization response function of the dipolar solvent using microscopic solvation models. The glassy nature of the protein-water interface breaks the direct link between the Stokes shift and the reorganization energy from equilibrium (ergodic) electron transfer theories. This suggests a mechanism that accounts for electron transfer in natural proteins, which are characterized by a low reaction free energy combined with a low activation barrier.

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