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The water effects on long-distance charge transfer in polypeptides NIKOLAI SERGUEEV, ALEXANDER DEMKOV, The University of Texas at Austin — Long-range electron transfer (ET) is one of the most intriguing reactions occurring in biological systems. Recent experiments indicate that water play an important role in the mechanism of charge transfer in proteins. In this talk we present the first-principles study of the effect of intervening water molecules on the electron tunneling processes in simple polypeptide bridges. The ET rate is related to the probability current that is computed using density functional theory and nonequilibrium Green's function formalism which takes into account the inelastic electron-phonon scattering in the bridge. Our results suggest that the effect of water is two fold. First, the insertion of water molecules changes the conformational and dynamic properties of the polypeptide molecule. Second, the presence of water modifies the electrostatics of the bridge. Both effects are found to have a significant effect on the electron transfer rate.

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