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Interprotein electron transfer through aqueous pathways JIANPING LIN, ILYA BALABIN, DAVID BERATAN, Duke University — Water contributes to tunneling mediation pathways as well as to reorganization energy in biological electron transfer. We examine the distance dependence of the inter-protein electron transfer through water at protein-protein interfaces by combining molecular dynamics (MD) and extended-Hückel analysis of cytochrome b5 self-exchange. Rather than describe the ET rate decay with a single exponential parameter, we employ explicit electronic structure calculations and find three distinct tunneling mediation regimes: a conventional protein-mediated regime at protein-protein contact, a "structured water" regime with soft distance dependence for small protein-protein gaps, and a bulk water regime with a rapidly decaying coupling at larger distance. Water density calculations also specify these three regimes. We calculate the bimolecular electron rate of cytochrome b_5 self-exchange system using Brownian dynamics with the multi-exponential decay electron transfer model built from these three regimes and the results are comparable with the experimental results within a factor of 5.

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