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A molecular breakwater enhances electron transfer between proteins NATHAN S. BABCOCK, University of Calgary, AURÉLIEN DE LA LANDE, Universite Paris-Sud, JAN ŘEZÁČ, Academy of Sciences of the Czech Republic, BARRY C. SANDERS, DENNIS R. SALAHUB, University of Calgary — Does natural selection optimize molecular biomachinery at the quantum level? We present statistical characterizations of molecular dynamics at an interprotein electron transfer (ET) interface. In simulations of the wild-type protein complex, we find that the most frequently occurring molecular configurations afford superior electronic coupling due to the consistent presence of a single water molecule hydrogen-bonded between the donor and acceptor sites. We attribute the persistence of this water bridge to a "molecular breakwater" composed of several hydrophobic residues surrounding the acceptor site. The breakwater supports the function of solvent-organizing residues by limiting the exchange of water molecules between the sterically constrained ET region and the surrounding bulk. When the breakwater is affected by a mutation, bulk solvent molecules disrupt the water bridge, resulting in reduced electronic coupling. These results suggest that protein surface residues may stabilize interprotein solvent dynamics to enable coherent ET along a single molecular pathway.

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