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Water-mediated energy transport and structure across a protein-protein interface DAVID LEITNER, University of Nevada, Reno — Water molecules embedded within proteins or at the interface between globules play a central role in folding and function. We discuss the influence of interfacial water molecules on energy transport and structure, specifically the role of water at the interface between the two globules of the homodimeric hemoglobin from Scapharca inaequivalvis, which binds oxygen cooperatively. We have studied the water-mediated energy transport in this protein with communication maps and nonequilibrium molecular simulations of energy flow, which reveal the disproportionate amount of energy carried by the water molecules, particularly across the interface, i.e., a larger thermal conductivity of the interfacial waters compared with other parts of the protein, promoting hydrogen bond rearrangements at the interface.

David Leitner
University of Nevada, Reno

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