

MIXED QUANTUM-CLASSICAL SIMULATIONS OF DISSIPATIVE PROCESSES IN PROTEINS

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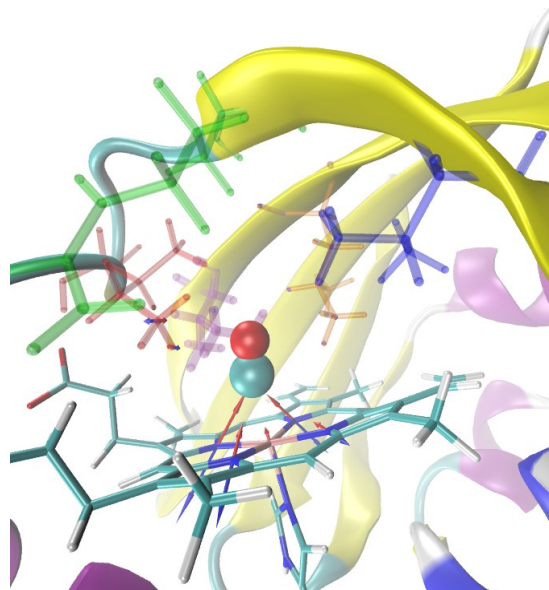
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We theoretically investigate dissipative processes of non-equilibrium systems by means of atomistic simulations. A mixed quantum-classical model is used comprising molecular dynamics (MD) and quantum dynamics based on mean field methods as well as vibrational surface hopping approaches. Thus an atomistic picture is obtained of environmentally-induced non-adiabatic transitions and decoherence phenomena. The quantum treatment provides access to state-resolved dissipation time scales. In particular, we show to what extent the simulated dynamical processes can be measured by nonlinear near-infrared spectroscopy and how certain observation directions yield valuable information on decoherence processes.

With respect to recent experiments [1], we study the IR active vibrational mode of a carbon monoxide molecule (quantum system) in the heme domain of the oxygen sensor protein FixL (classical system) in an aqueous environment. After photodissociation from the heme iron the unbound CO molecule remains vibrationally excited and floats into the heme pocket, where energy relaxation and quantum coherence decay occur.

A deeper understanding of dissipative processes and their influencing factors can provide better insights in energy transport phenomena in biological and artificial systems and opens thereby the possibility of their active control.



Unbound Carbonmonoxide in the FixL Heme pocket. Arrows illustrate the atomistic non-adiabatic coupling vectors for transitions to higher (red) or lower (blue) vibrational states of the CO.

[1] P. Nuernberger, K. F. Lee, A. Bonvalet, L. Bouzhir-Sima, J.-C. Lambry, U. Liebl, M. Joffre & M. H. Vos, *Journal of the American Chemical Society*, 133, 43 (2011), 17110-17113.