

Coherent Control of Long-range Photoinduced Electron Transfer by Stimulated X-ray Raman Processes

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We propose to use broadband X-ray pulses to control pathways and rates of long-range electron transfer (ET) in donor-bridge-acceptor (DBA) systems. Electron transfer between the donor, bridge and acceptor can be either enhanced or suppressed by stimulated X-ray Raman transitions resonant with selected core transitions. Simulations are carried out for a model Ru-Co light harvesting complex. Using the restricted excitation window time-dependent density functional theory (REW-TDDFT) and the generalized Redfield master equations we show how to vary the X-ray pulse parameters, such as shapes, phases and amplitudes, to achieve optimal control of electron transfer.