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Coherent quantum states in functionalized semiconductor nanostructures[1] LUIS G.C. REGO, Dept. of Physics, Univ. Fed. de Santa Catarina, SABAS ABUABARA, VICTOR S. BATISTA, Dept. of Chemistry, Yale University — We investigate the feasibility of creating and manipulating coherent quantum states in the surface of functionalized semiconductor nanostructures. Functionalization of a semiconductor nanocrystal can be achieved by anchoring organic ligands to its surface, with the resulting surface complexes often introducing electronic states in the band gap. These states sensitize the host material for photoabsorption, leading to photoinduced electron-hole pair separation and interfacial electron transfer to the semiconductor conduction band. A method that combines *ab-initio* molecular dynamics (MD) simulations with semi-empirical modelling reveals super-exchange hole tunnelling between adjacent catechol molecules adsorbed on TiO_2-anatase nanostructures. It is shown that electronic coherences can persist for hundreds of picoseconds, despite the partial intrinsic decoherence induced by thermal ionic motion usually observed in photoexcited semiconductor nanostructures. Moreover, the observed relaxation dynamics can be coherently controlled by a sequence of ultrashort 2π pulses. The proposed studies of decoherence and coherent optical control intend to explore the basic constituents of a molecular electro-optic device, based on inexpensive and easily manufacturable semiconductor materials.

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