Connecting quantum events to macroscopic phenomena: Multiscale simulation of photoresponsive materials

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A multiscale model for the simulation of a photoswitchable azobenzene-containing liquid crystal is presented, which links coarse-grained (CG) mesoscale simulations of the global structure to a nonadiabatic quantum-mechanical description of the local photoactive moiety via a classical atomistic model [1]. A nonadiabatic QM/MM approach has been developed [2, 3, 4] and applied to study the photoswitching of azobenzene in different environments — observing an increasing influence of the molecular surroundings going from vacuum, via an isotropic liquid, to an ordered liquid crystalline state. In the spirit of multiscale modelling, we have also developed a purely classical force field for photoswitching, based on the quantum data, that enables us to study a high density of photoisomerisation events and their impact on the liquid crystalline order. In order to gain access to mesoscopic time and length scales on which liquid crystalline phase transitions take place, coarse grained simulation models are used, with substantially fewer degrees of freedom compared to an all-atom level of resolution.

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