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From Computational Photobiology to the Design of Vibrationally Coherent Molecular Devices and Motors

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In the past multi-configurational quantum chemical computations coupled with molecular mechanics force fields have been employed to investigate spectroscopic, thermal and photochemical properties of visual pigments. [1,2] Here we show how the same computational technology can nowadays be used to design, characterize and ultimately, prepare light-driven molecular switches which mimics the photophysics of the visual pigment bovine rhodopsin (Rh) [2,3]. When embedded in the protein cavity the chromophore of Rh undergoes an ultrafast and coherent photoisomerization. In order to design a synthetic chromophore displaying similar properties in common solvents, we recently focused on indanylidene-pyrroline (NAIP) systems. [3,4] We found that these systems display light-induced ground state coherent vibrational motion similar to the one detected in Rh. Semi-classical trajectories provide a mechanistic description of the structural changes associated to the observed coherent motion which is shown to be ultimately due to periodic changes in the π-conjugation.

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