A Sequential-QM/MM study of the electronic spectra of the dihydroazulene/Vinylheptafulvene molecular switch

Marcelo Hidalgo Cardenuto[1], **Sylvio Canuto**[1]

[1]*Instituto de Física, Universidade de São Paulo, São Paulo, Brasil*

In this work we present a theoretical study of a photochromic molecular switch. The target molecule is composed by two units of the dihydroazulene (DHA)/Vinylheptafulvene (VHF) covalently linked by a benzene ring. We use a sequential Quantum Mechanics/Molecular Mechanics (S-QMMM) methodology to investigate the solvent effects on the electronic spectra of these molecules. Four isomers of this molecule are studied depending on the open/close forms of the DHA/VHF unit. Classical Monte Carlo simulations are performed to obtain the liquid structures of the solvent and then quantum mechanics calculations are used to obtain the electronic spectra at Density Functional Theory level. The solvent effect is considered both as an electrostatic embedding composed by the point charges of the solvent molecules (acetonitrile) as well as the closest explicit acetonitrile molecules. The shifts of the absorption band in relation to the isolated molecules are calculated and the inhomogeneous broadening are obtained in good agreement with the experiment.