Computational modelling of switchable organic materials

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Compounds which undergo reduction and oxidation reactions, especially at relatively low energies, can serve as switches and other components in electronic devices. Large, conjugated organic molecules which can form stable redox products can also present additional interesting optoelectronic properties such as second harmonic generation (generating frequencies of light other than those that the sample is exposed to) and other nonlinear optical (NLO) effects.

The molecule we are studying is a synthetic conjugated organic compound which due to conjugation and aromaticity is a target for both of these applications. It is optically active due to its conjugation, and it has two oxidation states besides the ground state. Successive oxidation of the compound gives first a radical cation and then a diradical dication.

Using computational methods we have studied the molecular geometries of each oxidation state of this molecule. We have also studied many of the properties of the molecule and its cations to explain its electrochromic behaviour (changing colour ion oxidation). We computationally modelled the polarity and multipole expansions, as well as the frequency responses (IR and raman spectra).

Given the standard phase of this compound is solid, we are studying the crystal structure and the properties in the crystal phase at the moment. This involves attempting to find a optimal crystal structure, and performing computational calculations on these structures. A further step we are taking in an attempt to find a proper crystal structure is doing geometry optimization of dimer and other small clusters of molecules in order to gain insights to the interactions of these molecules in order to aid generation of a unit cell for the crystal structure.