DFT applications to CD and absorption-phosphorescence spectroscopy.

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Results will be presented regarding two DFT spectroscopic studies we recently started. In the first one, we deal with two DFT Ru(II) antenna complexes, one of them showing dual emission and the other a lack of it. We started with geometry optimizations for the ground and excited state structures, using TDDFT. From the optimized geometries, we evaluated vertical excitation energies and oscillator strenghts in order to get the absorption spectra. We took into account the most intense excitations that involve charge transfer from the Ru atom to the ligands to carry out the corresponding excited state geometry optimizations. From the minima of these singlet excited states, we considered the possible emission spectra.
To get insight into singlet-triplet transitions, we obtained the appropriate spin-orbit coupling integrals. In order to study phosphorescence, we additionally optimized the geometries of the two first triplet excited states, and evaluated vertical emission spectra. Spin-orbit coupling elements and electric dipole transition moments were also considered in the analysis. Radiative phosphorescence lifetimes for the three spin sublevels, and in the high temperature limit were computed.
In the second study, we evaluated CD spectra of several poly(phenylacetylene)s in order to be able to determine their helical sense. We started with geometry optimizations, and determined the dependence of the CD spectra with the number of phenylacetylene units. Additionally, several substituents were considered and their influence on the polymer helical sense was studied.
To optimize geometries and calculate absorption and emission spectra, we used the Gaussian 09 program, and for spin-orbit coupling constants, dipole moment integrals, and CD spectra DALTON.