**Link:** <https://solar-power-tech.com/e-posters/dsc_eposter_15/>

**Abstract**

Curcumin is a natural compound known for its antioxidant and antitumor properties [1]. Although it is already applied as a dye in photodynamic therapy, it has not been tested yet for energy conversion purposes. Curcumin molecule presents an extended pi-conjugated system, ideal for electron conduction applications, and presents absorption transitions mainly in the UV-visible region of the electromagnetic spectrum.

Different organic anchoring groups and several coordinated transition metals have been evaluated regarding their influence on pure curcumin’s absorption spectra. Simulations were made using calculation methods based on the Density Functional Theory [2,3], with B3LYP/6-31G level for optimizing the organic portion of the structures and B3LYP/LANL2DZ for complexes with heavy metals. For further exploration into the excited states, the time-dependent DFT (TD-DFT) method was employed with varied functionals, each of them including a different Hartree-Fock electronic exchange percentage.

Regarding the organic anchoring groups, minimum blueshifts were obtained in absorption peaks, mainly in the UV-Visible region. Results for metal complexes indicate potential charge transfers between curcumin and metal ions - which is an essential feature for dyes, as the excited electrons must travel through the species to reach the semiconductor’s conduction band. The spectra present wide absorption bands, including in the visible region, and show red-shifted peaks when compared to the pure curcumin spectrum. All results are in good agreement with previous theoretical and experimental works available in the literature [4] and indicate curcumin as a potential candidate for cheap and non-toxic applications as DSSC’s dyes.