Electronic Structure-Property Relations of Photochromic MOFs from the Cambridge Crystallographic Structural Database

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The photochromic characteristics, the reversible color change upon UV irradiation is common in pyridinium-based MOFs, and it has tremendous applications in various fields such as stimuli-responsive adsorption, modulation of emission colors, controlled reversible singlet oxygen generation, and inkless and erasable printing media, etc. Albeit the structural features responsible for the photochromic behavior in the viologens-based MOFs is well documented in the literature, the underlying mechanism for the donor-acceptor charge transfer is not yet established concerning the geometrical parameters. Understanding the electronic structure-based charge-transfer mechanism would enable the fine tuning of the photochromic applications. To execute the computation, a photochromic MOF database was created from the MOF-subset of CCDC, and time-depended density functional theory (TD-DFT) was used to comprehend these charge transfer mechanism through analyzing the appropriate excited state frontier molecular/crystal orbitals (FM/CO), and it account for the structure-property relationships.