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Tuning energy level alignment at organic/semiconductor interfaces using a built-in dipole in Chromophore-Bridge-Anchor compounds

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— We report a new approach, using chromophore-containing molecules designed to contain internal dipoles, for controlling at the molecular level the energy level alignment between an organic chromophore and a transition metal oxide surface. The approach employs a chromophore-bridge-anchor molecular architecture where the three components are electronically decoupled. By introducing electron donor (D) and acceptor (A) groups to the bridge, an intramolecular dipole is introduced between the chromophore and the anchor. When a monolayer of such molecules is bonded to a metal oxide surface, the resulting dipole layer establishes a potential difference that shifts the chromophore levels with respect to those of the substrate. This concept is demonstrated using a chromophore (ZnTPP)-bridge (substituted with an electron donating (NMe2) and electron withdrawing (NO2) groups to create a built-in dipole)-anchor (Isophtalic acid) architecture. Shifts of the chromophore's HOMOs on the order of plus or minus 0.1 eV with respect to the ZnO valence band edge have been observed, without altering the photoabsorption properties of the chromophore or the HOMO-LUMO gap. An important strength of this concept is that it provides a general design applicable to a large number of anchoring functional groups, built-in dipole bridges, and redox-active centers.

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