Supporting Information

Density Functional Theory Design of Double Donor Dyes and Electron Transfer on Dyes/TiO_2(101) Composites Systems for Dye-Sensitized Solar Cells

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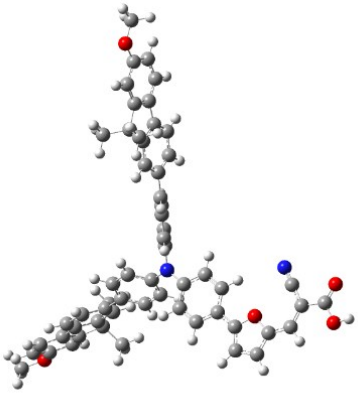
ME101



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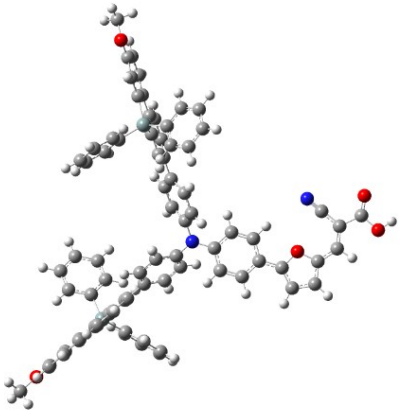

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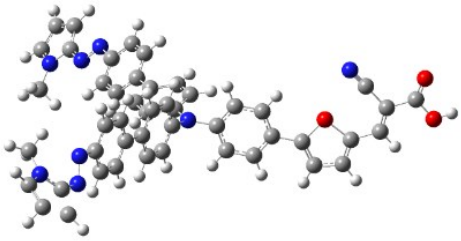

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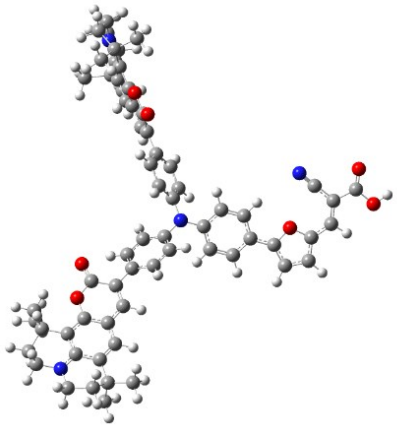

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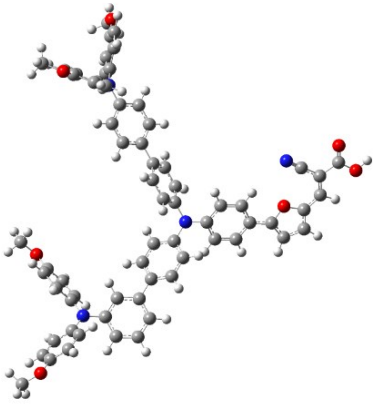

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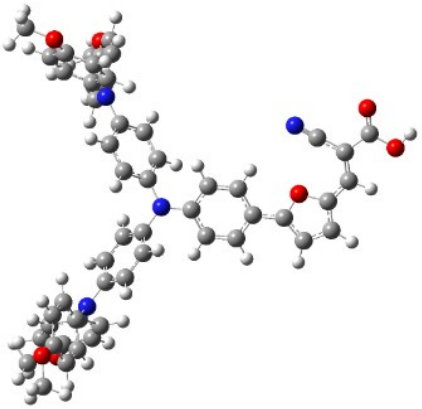


WD8

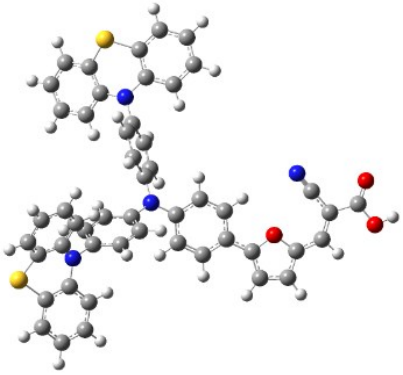
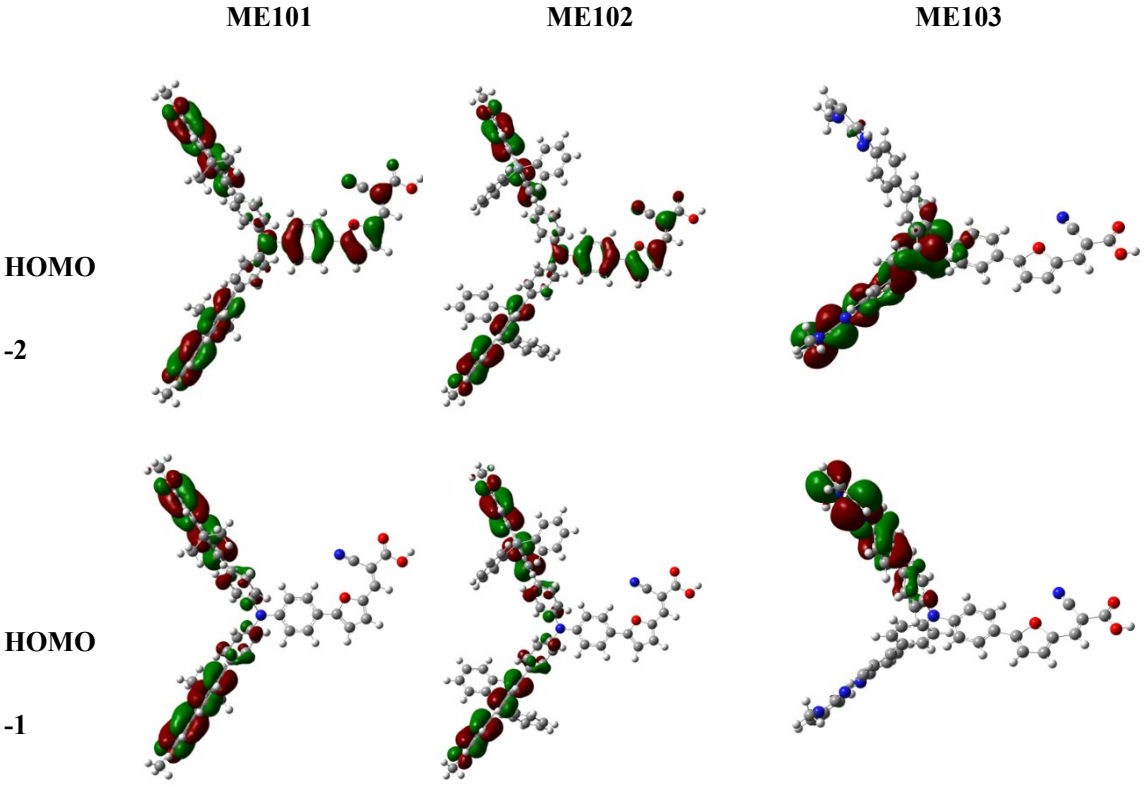
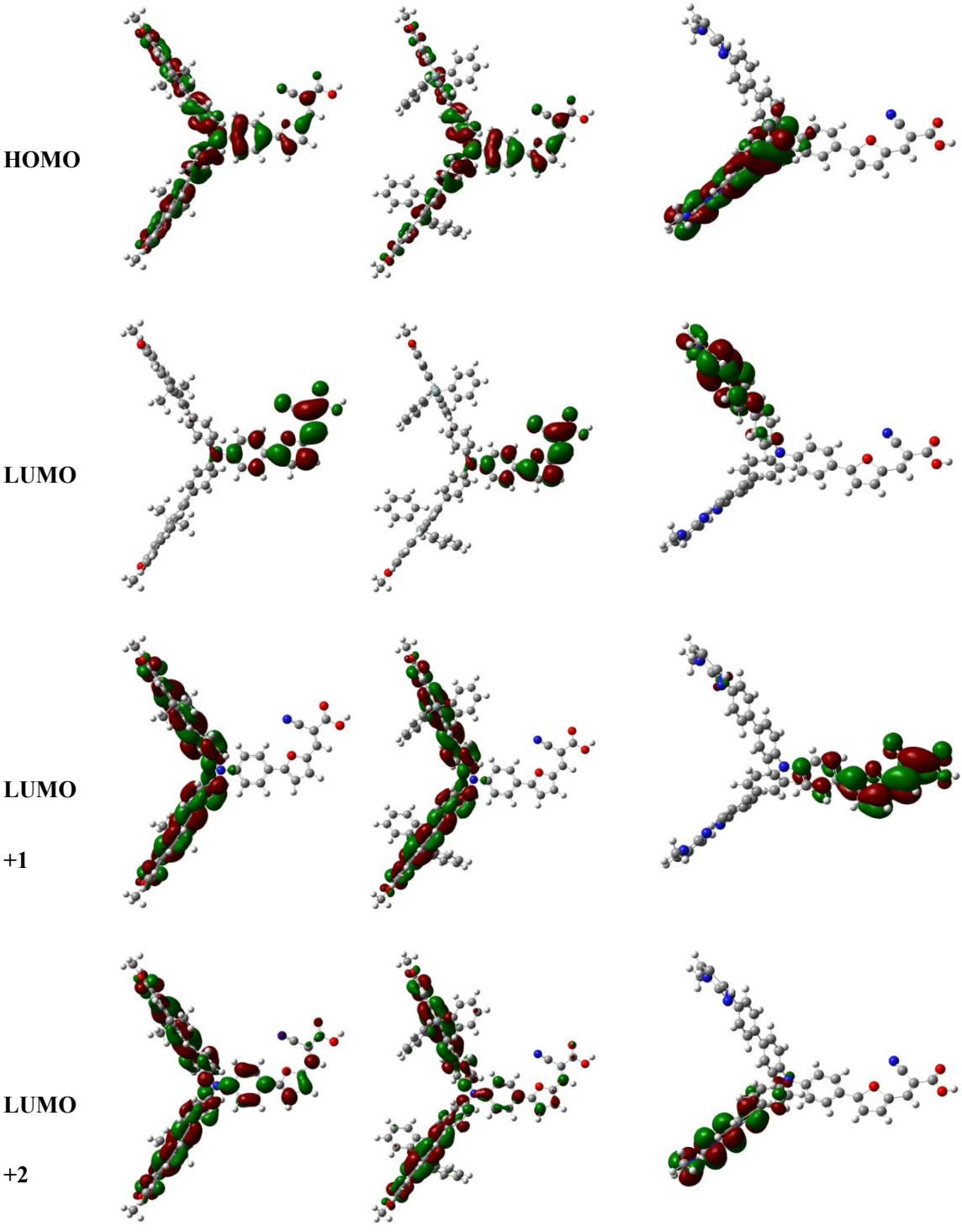
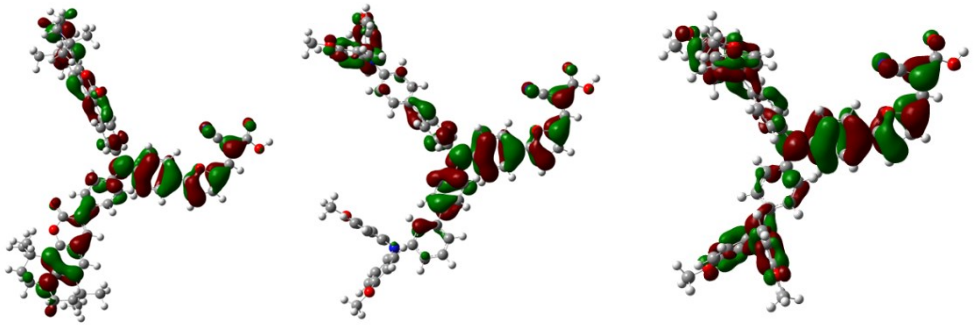


Fig. S1**.** The optimized structures of **ME101-ME106 and WD8.** Gray, red, yellow, blue, purple, and white spheres represent C, O, S, N, Si and H atoms, respectively

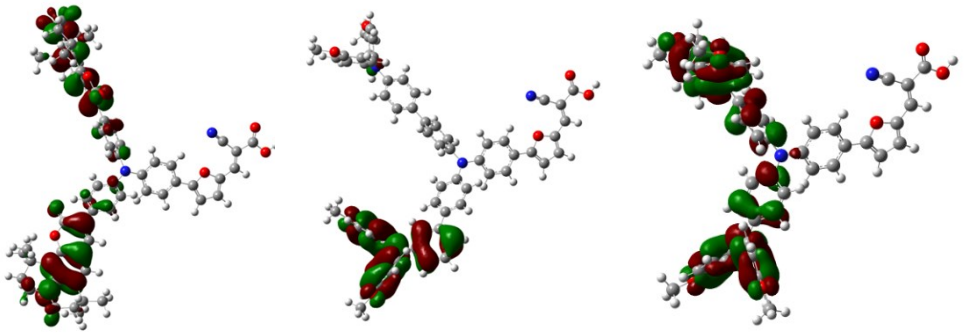



HOMO
LUMO
LUMO
+1
LUMO
+2
ME104
ME105
ME106

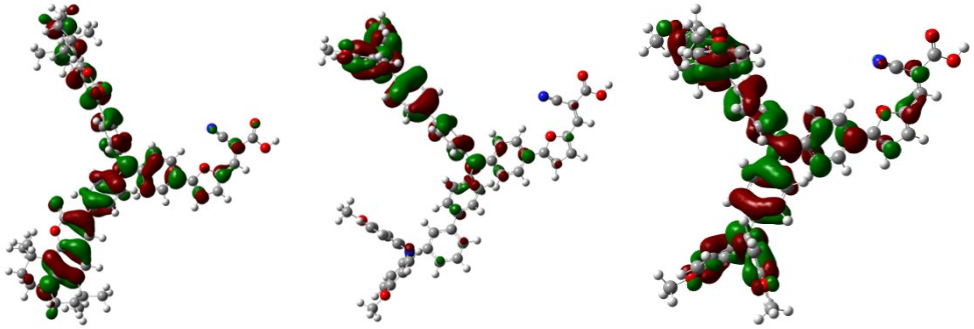
HOMO -2



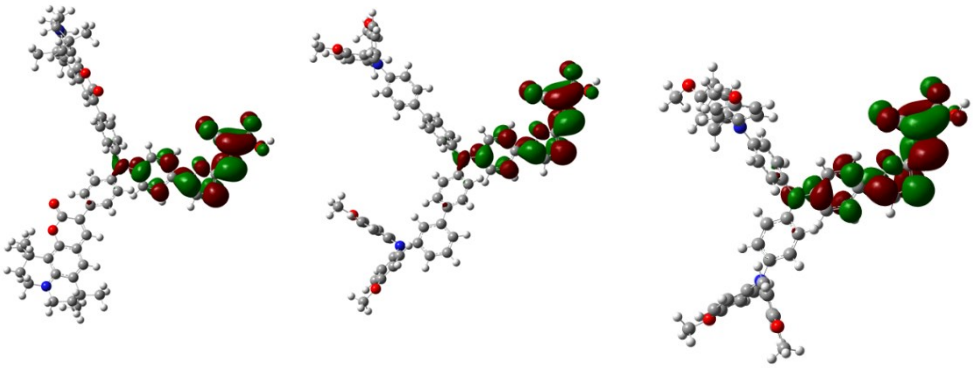
HOMO -1



HOMO



LUMO



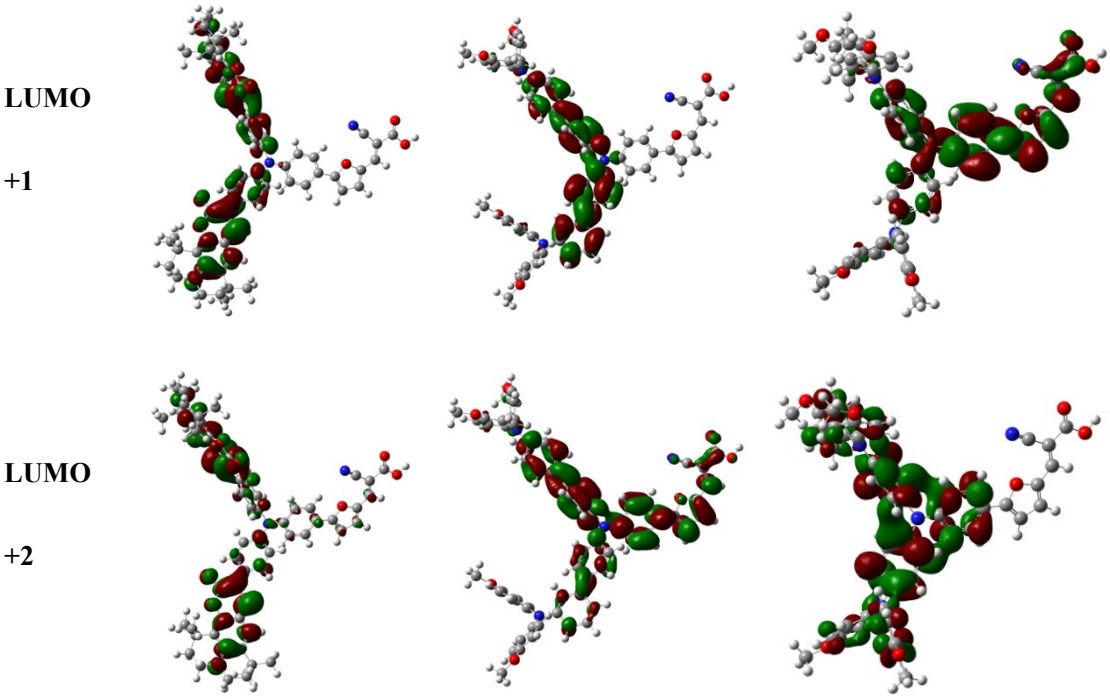
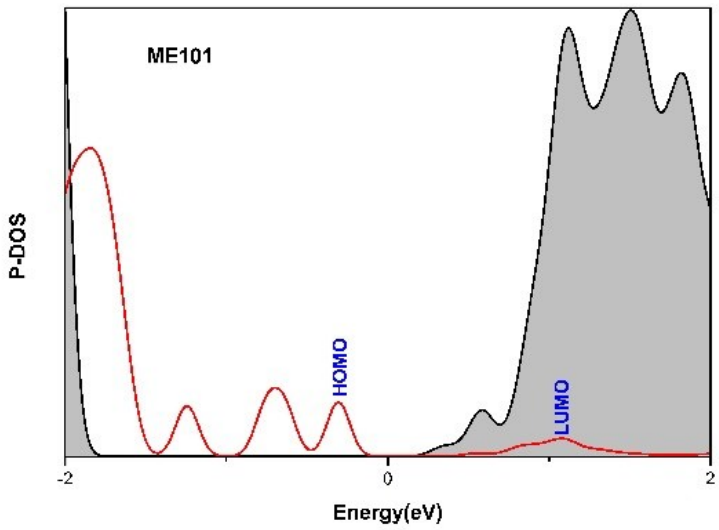
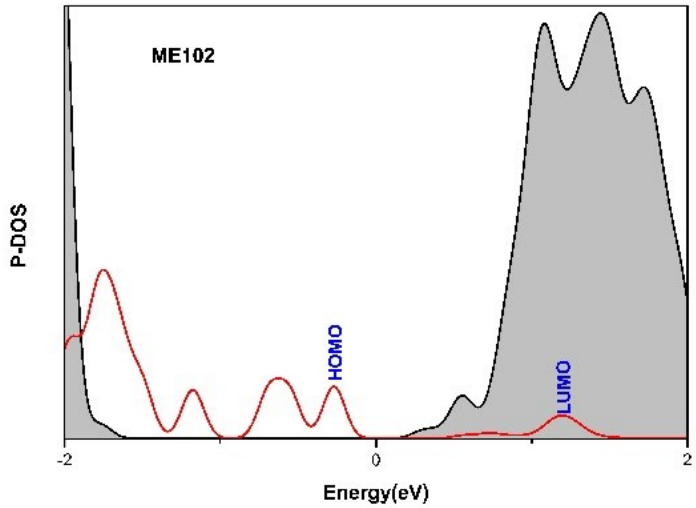
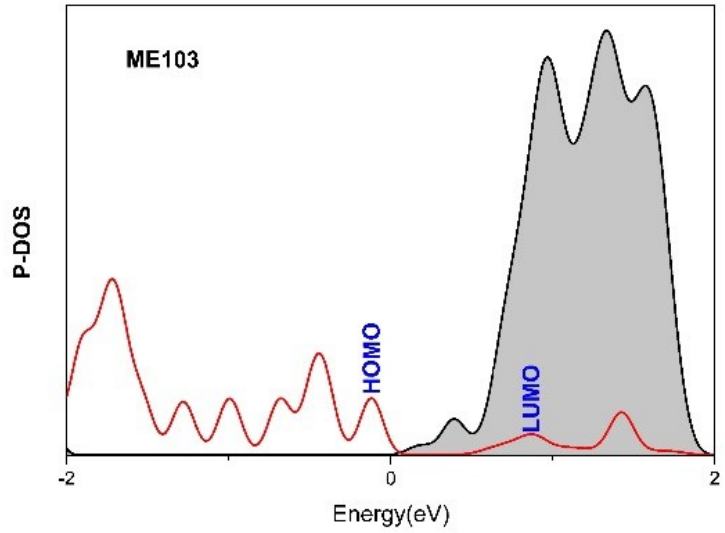
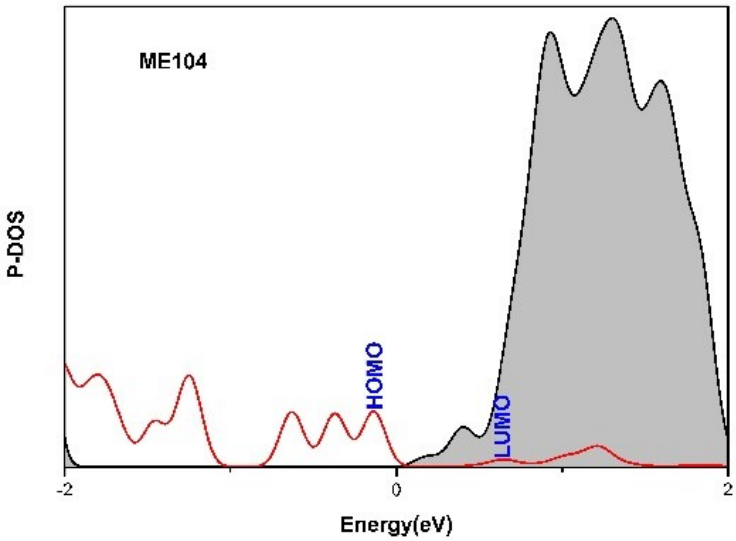


Fig. S2. Frontier molecular orbitals of **ME101-ME106**.




ME102
P-DOS
HOMO
LUMO
-2
0
2
Energy(eV)


ME103
P-DOS
HOMO
LUMO
-2
0
2
Energy(eV)


ME104
P-DOS
HOMO
LUMO
-2
0
2
Energy(eV)

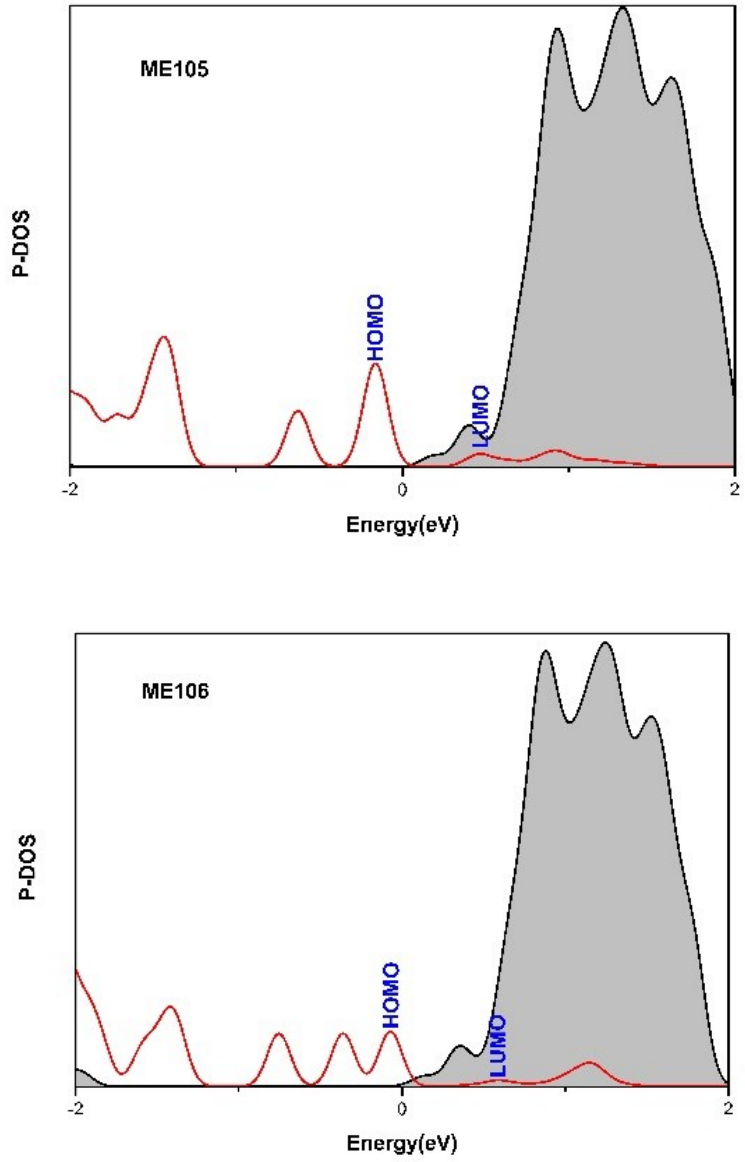


Fig.S3 Calculated projected density of states for **ME101-ME106**. Red curves are for the dyes and the black lines are for the TiO_2 substrate

Calculation Methods of Absorption Spectra

The spectrum is obtained using the following expression [1] base on the calculated excitation energies (ω_I) and oscillator strengths (f_1)

$$\varepsilon(\omega) = 2.174 \times 10^8 \sum_I \frac{f_I}{\Delta} \exp\left[-2.773 \frac{(\omega - \omega_I)^2}{\Delta^2}\right] \quad (1)$$

where the molar extinction coefficient is given in units of $M^{-1}cm^{-1}$, the energies ω,

$\omega_I$and Gaussian full-bandwidth at half-height are expressed in cm^{-1}, and f_I is the corresponding oscillator strength. This expression satisfies the well-known relationship

$$4.32 \times 10^{-9} \int \varepsilon(\omega) d\omega = \sum_I f_I \qquad (2)$$

We use =4000cm^{-1} for the optical band broadening to mimic thermal oscillations in dye structures and excitations at room temperature, which is very close to those in experimentally measured absorption spectra.

The molar extinction coefficients calculated from eq1 are comparable to experimentally measured ones [2] after applying an overall scaling factor of ~0.5 for the size of the peaks.

[1] Hay, P.J. and W.R. Wadt.J Chem Phys, 1985. **82**(1) 270-283.
[2] Zhang, G., et al.Chem Commun, 2009(16): 2198-2200.