

Supporting Information for:

Tuned Hydrogen Bonding in Rare Earth MOFs for Design of Optical and Electronic Properties: An Exemplar Study of Y-DOBDC

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Table S1. Total number of H-bonds for each H-bonding configuration % and on which type of ligand the H-bonds are located.

H-Bonding %	Number of H-bonds	Monodentate H-Bonds	Bidentate H-Bonds
0	0	0	0
20	4	4	0
40	8	0	8
60	12	4	8
80	16	0	16
100	20	4	16

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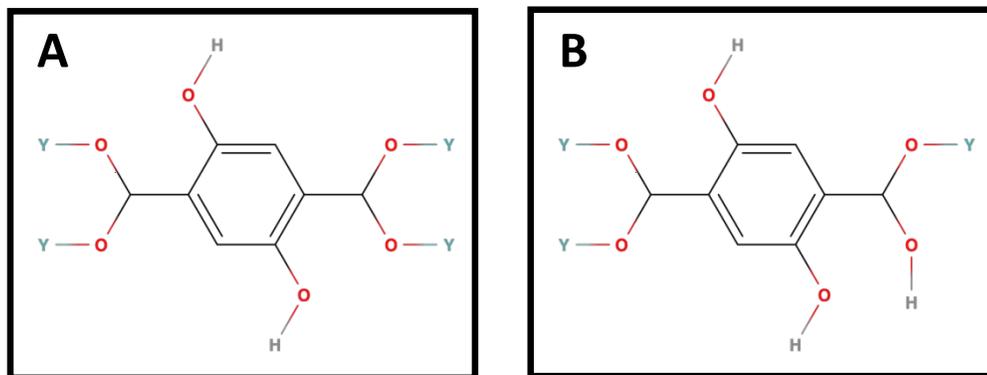


Figure S1. Two binding structures of the DOBDC linkers to the metal clusters in a (A) bidentate and (B) monodentate fashion.

Table S2. Calculated total energies and calculated average H-bond strength of isolated H₄-DOBDC.

H-Bonding Configuration	Total Energy (eV)	H-Bond Strength	kJ/mol
Interacting	-140.02	E_{IHB}	27.75
Not Interacting	-139.44		

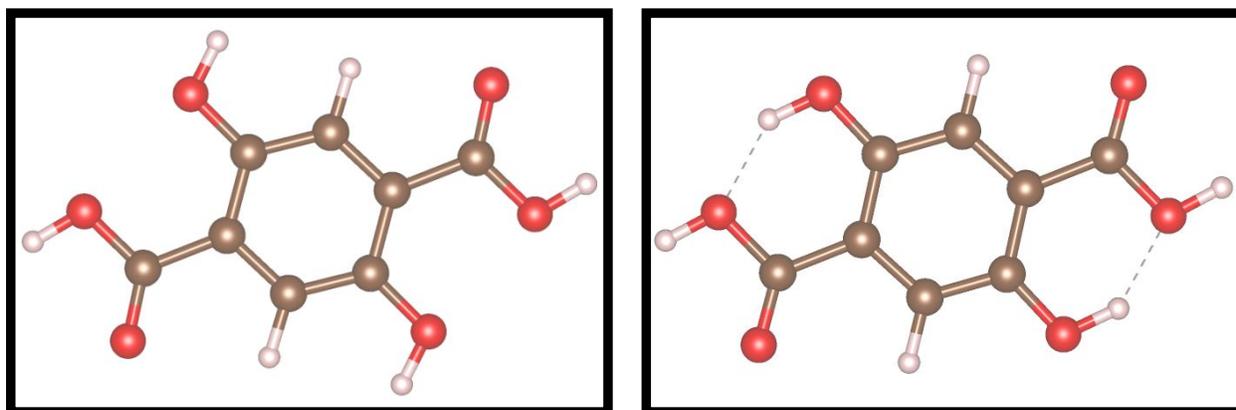


Figure S2. Calculated optimized geometries of isolated H₄-DOBDC molecules with no H-bonding (left) and H-bonding (right). Colors: H (white), O (red), C (grey)

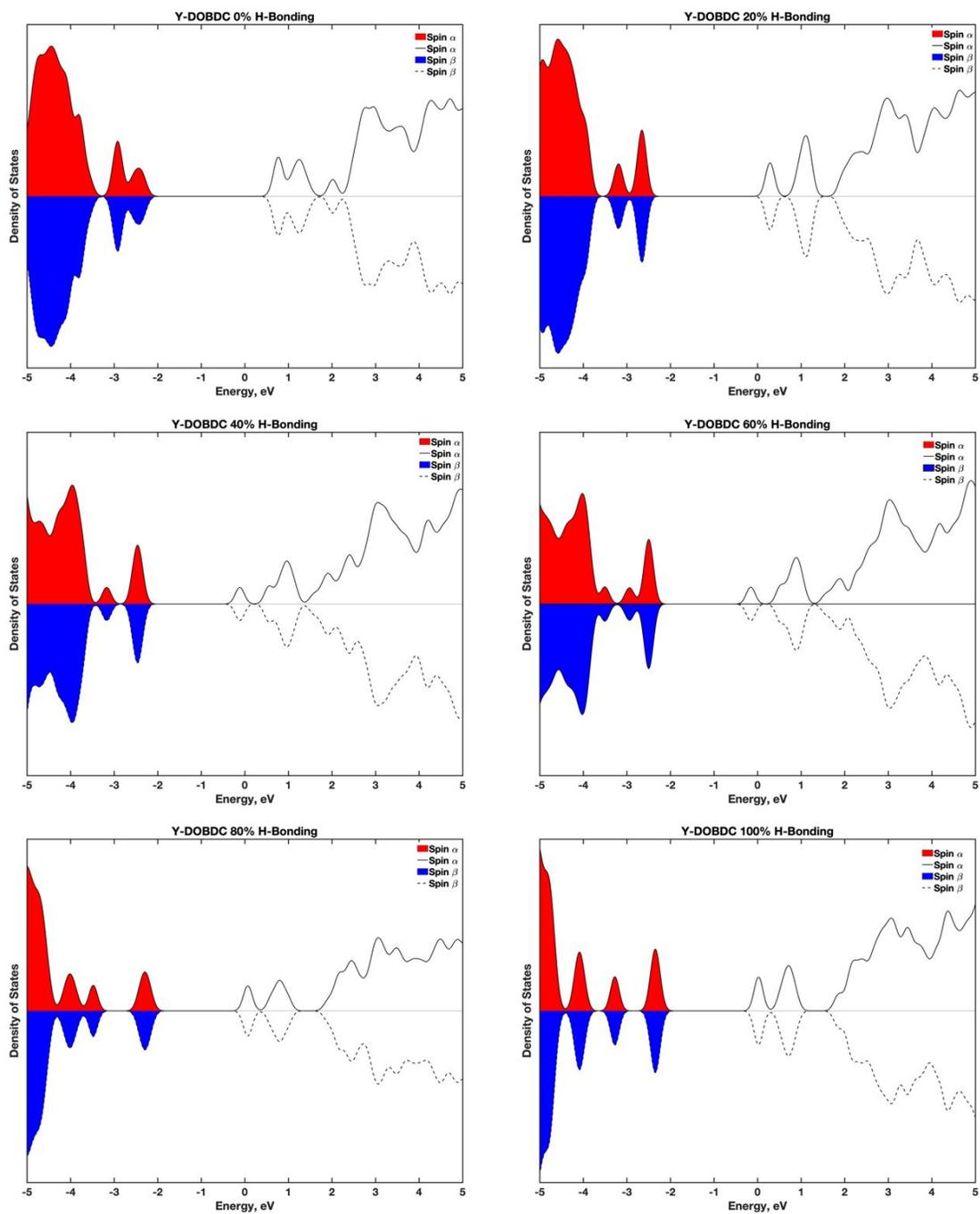


Figure S3. Calculated density of states for Y-DOBDC with H-bonding configurations from 0-100% using HSE06. Occupied (shaded) and unoccupied (unshaded) electronic states are plotted for both the spin alpha (red/solid line) and spin beta (blue/dotted line) projections.

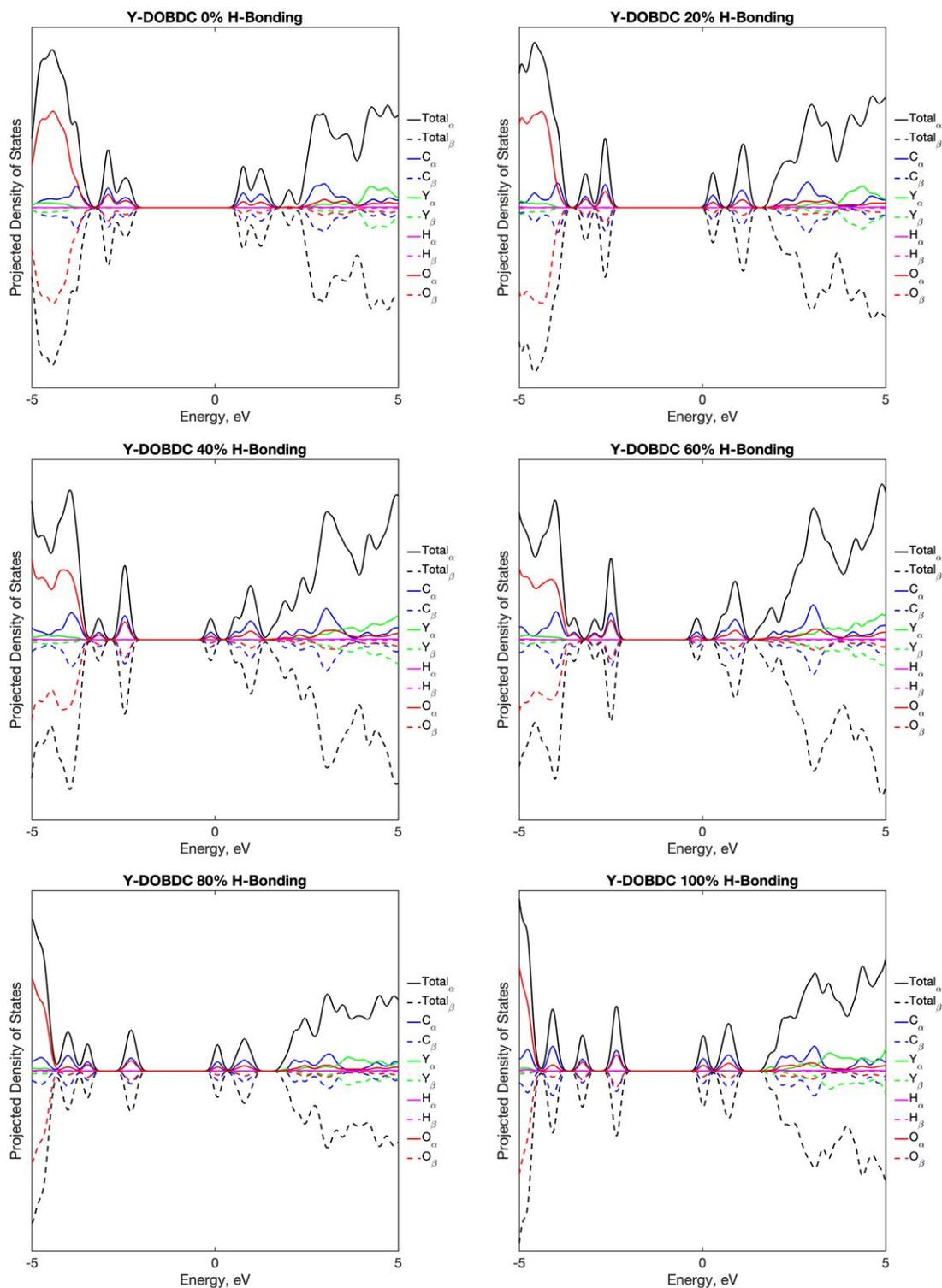


Figure S4. Projected density of states (PDOS) for Y-DOBDC with H-bonding configurations from 0-100%, calculated with the HSE06 hybrid functional. Each PDOS plot provides the total DOS (black) and the contribution of the individual elements: C (blue), Y (green), O (red), H (pink). Each PDOS is plotted for both the spin up (solid lines) and spin down (dashed lines) projection.

Calculated optical spectra.

The DFT calculated ground state electronic structures provide solutions to solving the one electron Kohn-Sham (KS) equation in the form of Kohn-Sham orbitals (KSOs), $\varphi_{\sigma,i}^{KS}$, and their respective energies, $\varepsilon_{i,\sigma}$. The use of spin unrestricted DFT provides solutions for both spin up (α) and spin down (β) projections, indicated by σ . From the calculated KSOs the transition dipole moment can be calculated with spin conservation in the independent orbital approximation between two states i and j , $\vec{D}_{\sigma,ij} = e \int \varphi_{\sigma,i}^{KS*} \vec{r} \varphi_{\sigma,j}^{KS} d\vec{r}$. The transition dipole moment is then used to calculate the oscillator strength, $f_{\sigma,ij}$, for the transition ij , as $f_{\sigma,ij} = |\vec{D}_{\sigma,ij}|^2 \frac{24\pi m_e \omega_{ij}}{3\hbar e^2}$, where ω_{ij} is the energy of the transition. The oscillator strength is used to weight the absorption of the transition, $a_{\sigma,ij}$, allowing for the calculation of the absorption spectrum as $a_{\sigma}(\varepsilon) = \sum_{\sigma,ij} f_{\sigma,ij} \delta(\varepsilon - \Delta\varepsilon_{\sigma,ij})$; $a(\varepsilon) = a_{\alpha} + a_{\beta}$.