Supporting Information

Amorphous covalent inorganic-organic hybrid frameworks (CIOFs) with an aggregation induced selective response to UV-visible light and their DFT studies

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Quantum calculation methods in materials studio

The crystal structures (HCCP, BPS, and TATA) for the density functional theory (DFT) and first-principle calculations were obtained from the PubChem database (https://pubchem.ncbi.nlm.nih.gov). The plane wave DFT calculation conducted using the Cambridge Sequential Total Energy Package (CASTEP) packaged in Materials studio 2017 (BIOVIA) (https://www.3dsbiovia.com/products/datasheets/castep.pdf).[1] The exchange-correlation functional under the generalized gradient approximation (GGA)[2] was used as exchange-correlation functional with norm-conserving pseudopotentials. The describe the electron-electron interaction Perdew-Burke-Ernzerh (PBE) was implemented as functional.[3] Materials Studio DMoL3 was used to optimize the ground state geometries in the gaseous state by

using GGA as an exchange-correlation function for all electrons.[4] DNP basis set 4.4 was used with for all-electron calculations. The PBE functional was used with fine quality. The electron densities were visualized in Materials Studio. DMoL[3] achieves its speed and accuracy by using numerical functions (https://www.3dsbiovia.com/products/datasheets/dmol3.pdf) on an atom-centered grid as its atomic basis. The DFT equations can be solved for the individual atoms to get the atomic basis functions so it is quite accurate.

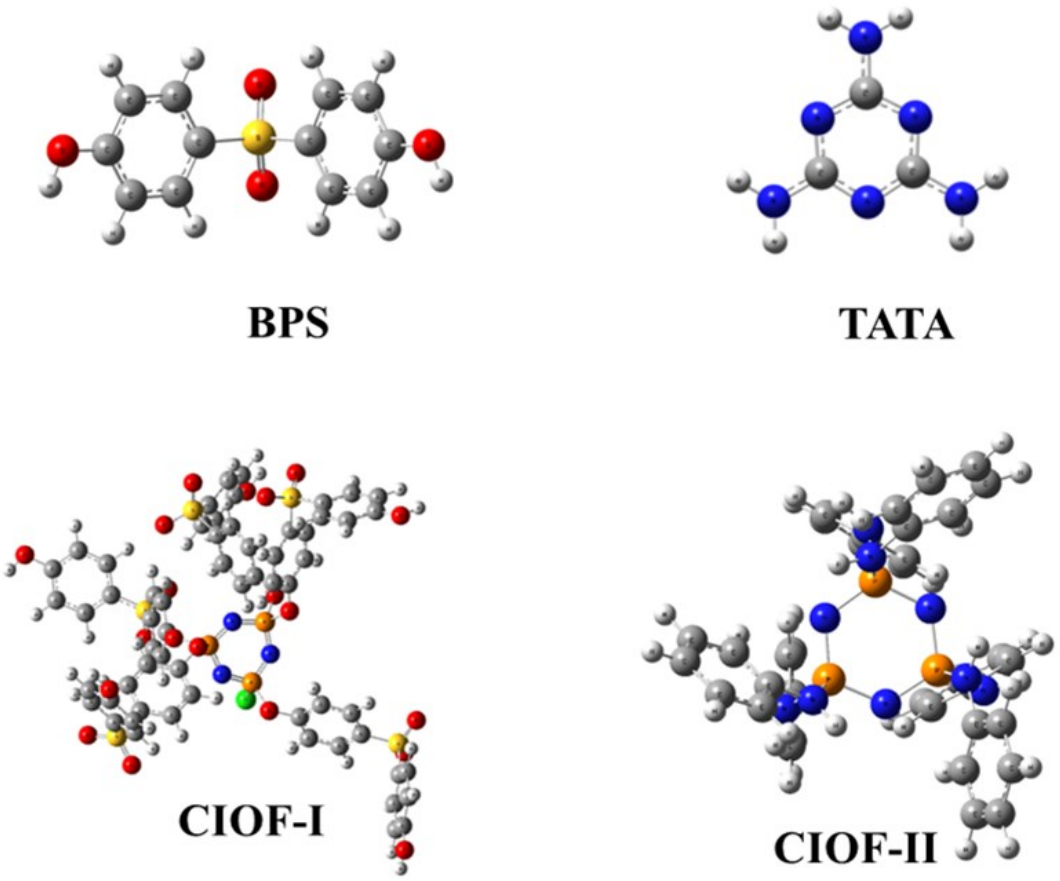

Fig. S1. Optimized structures of BPS, TATA, and their derived CIOF-I and CIOF-II at B3LYP/6–311+G*(d,p)* level on Gaussian 09.

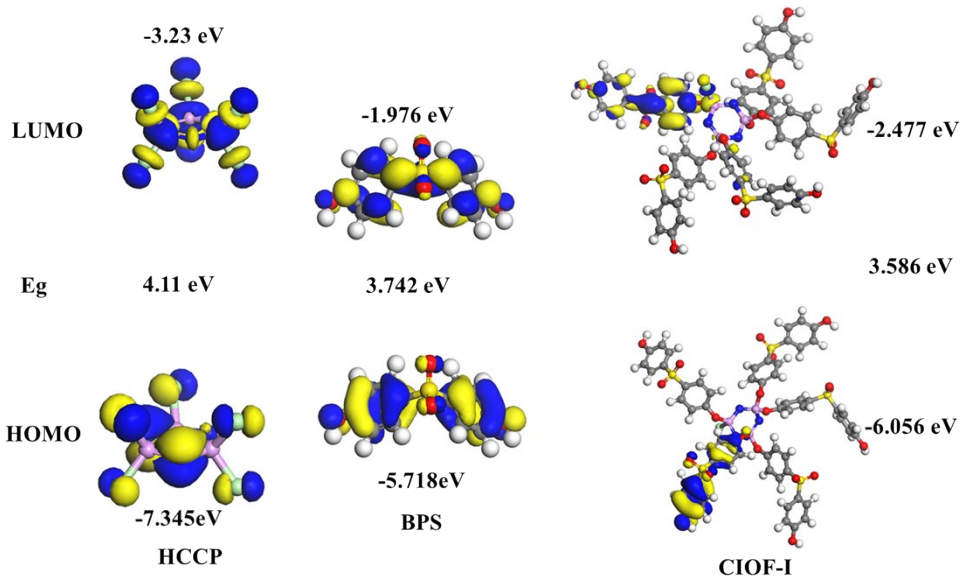

Fig. S2. Optimized structure for HCCP, BPS, and CIOF-I along with their frontier electron densities and their potentials calculated by using GGA/PBE/DNP 4.4 basis set on DMoL^3 DFT package in Materials Studio.

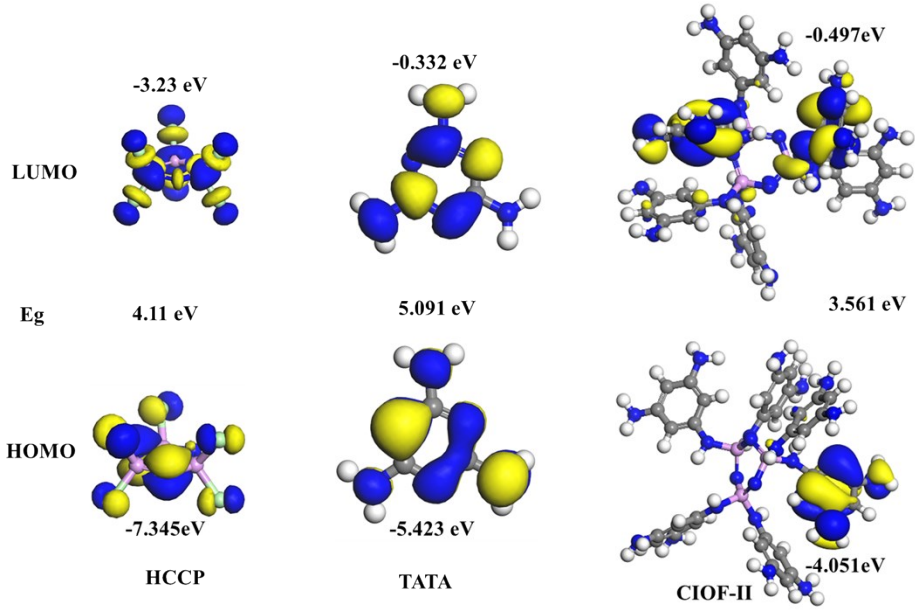

Fig. S3. Optimized structure for HCCP, TATA, and CIOF-II along with their frontier electron densities and their potentials calculated by using GGA/PBE/DNP 4.4 basis set on DMoL^3 DFT package in Materials Studio.

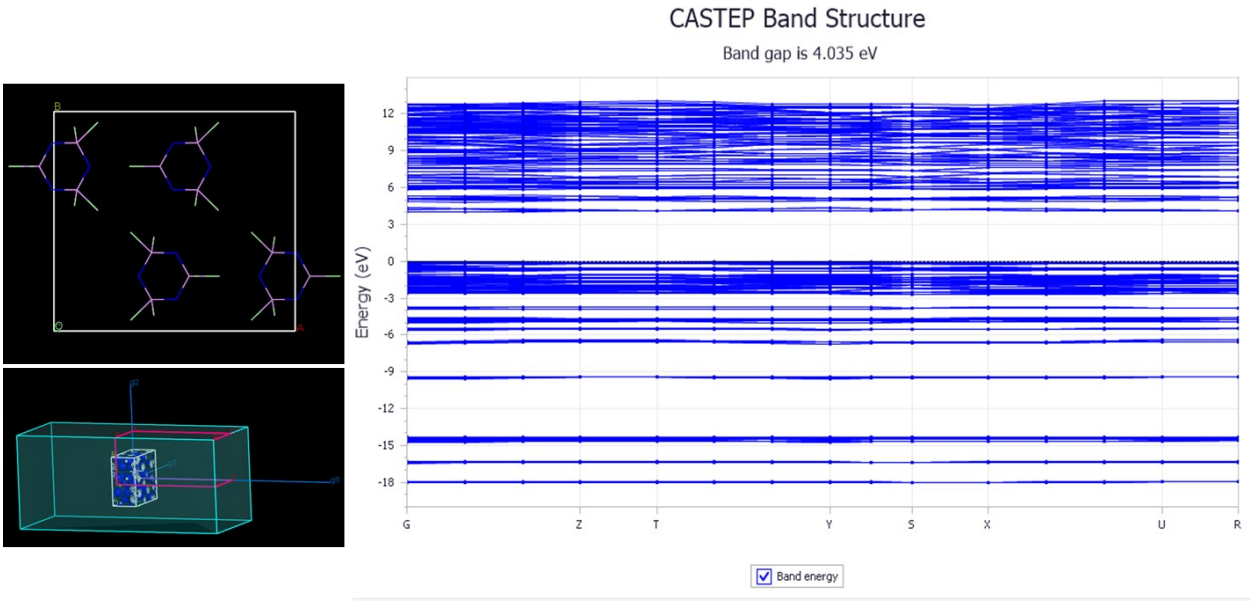

Fig. S4. The optimized crystal structure for HCCP (obtained from PubChem database) with electron densities and their band structure calculated by using the CASTEP Plane Wave DFT package in Materials Studio.

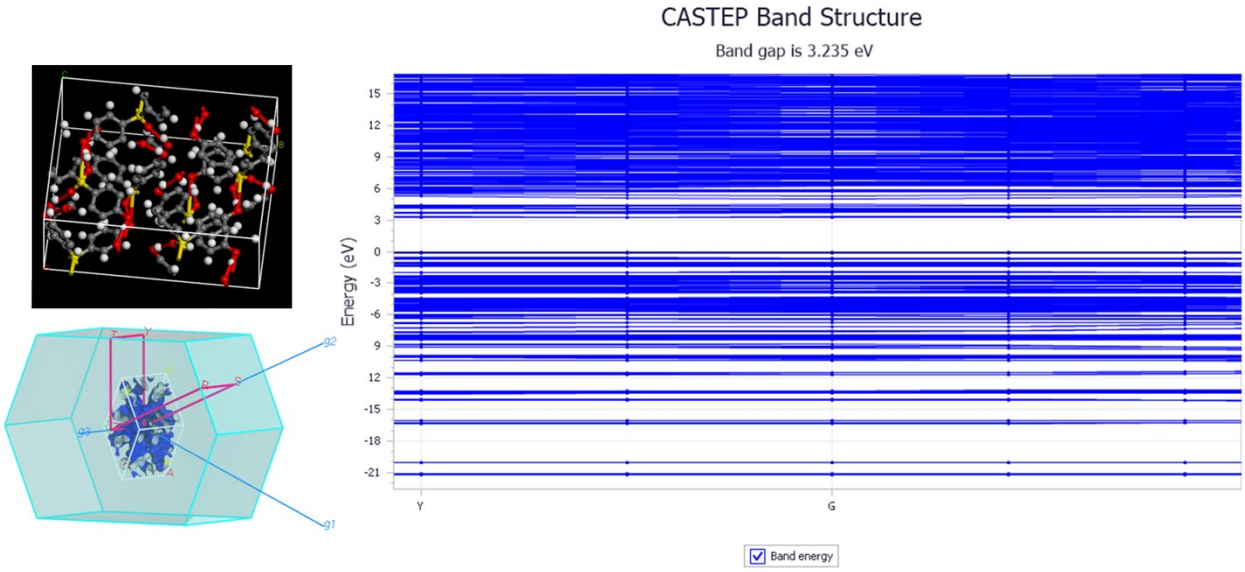

Fig. S5. The optimized crystal structure for BPS (obtained from PubChem database) with electron densities and their band structure calculated by using the CASTEP Plane Wave DFT package in Materials Studio.

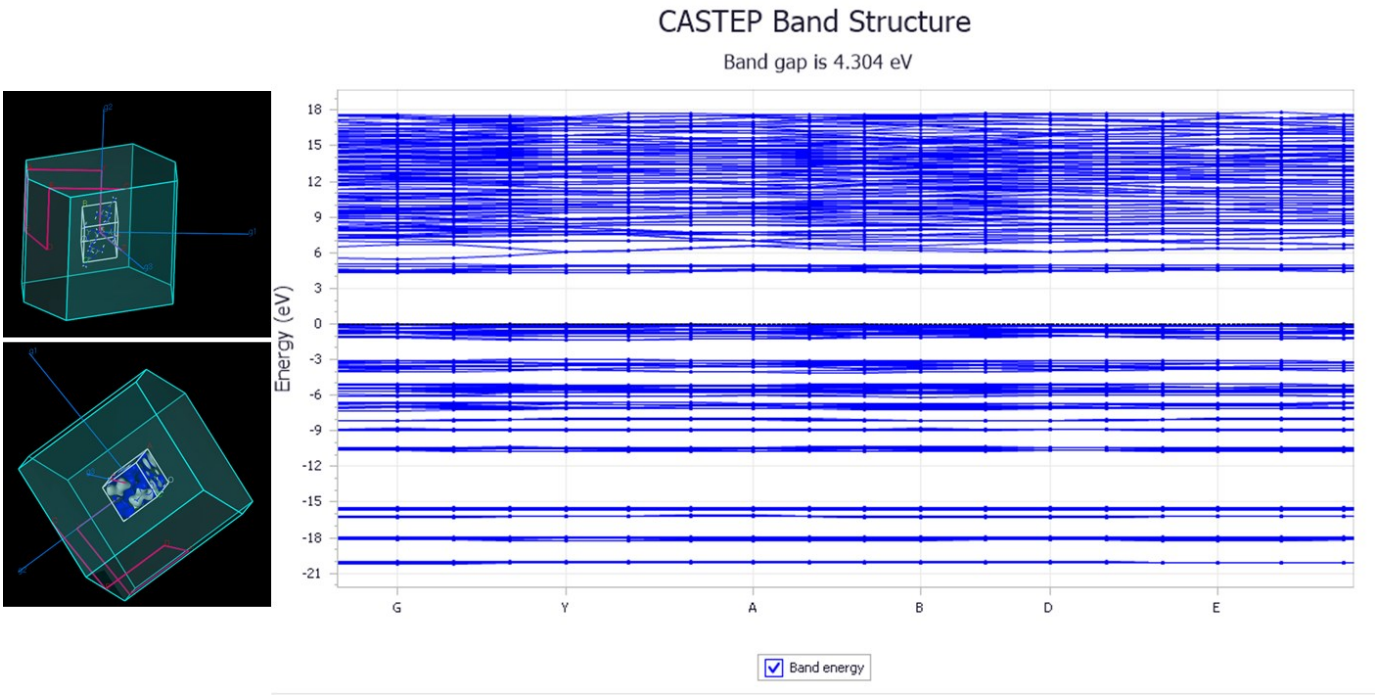

Fig. S6. The optimized crystal structure for TATA (obtained from PubChem database) with electron densities and their band structure calculated by using the CASTEP Plane Wave DFT package in Materials Studio.

Table S1. Comparison of the different computational methods used for the determination of Eg along with the experimental values.

	Gaussian 09 B3LYP/6–311+G (d,p) (Eg eV)	**DMoL^3 GGA/PBE/DNP/4.4/Fine (Eg eV)**	**CASTEP GGA/PBE/Norm-conserving (crystal form) (Eg eV)**	**Experimental Eg (eV) from Absorbance edge**
HCCP[5]	5.745	4.11	4.035	4.80
BPS	4.05	eV	3.325	3.79
TATA	4.79	5.091	4.30	4.25
CIOF-I	3.92	3.586	----------	3.84
CIOF-II	3.89	3.561 eV	----------	3.81

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