Electronic Supplementary Information

Metal-Organic Kagome Lattices M_3(2, 3, 6, 7, 10, 11-hexaiminotriphenylene)$_2$ (M = Ni and Cu): From Semiconducting to Metallic by Metal Substitution

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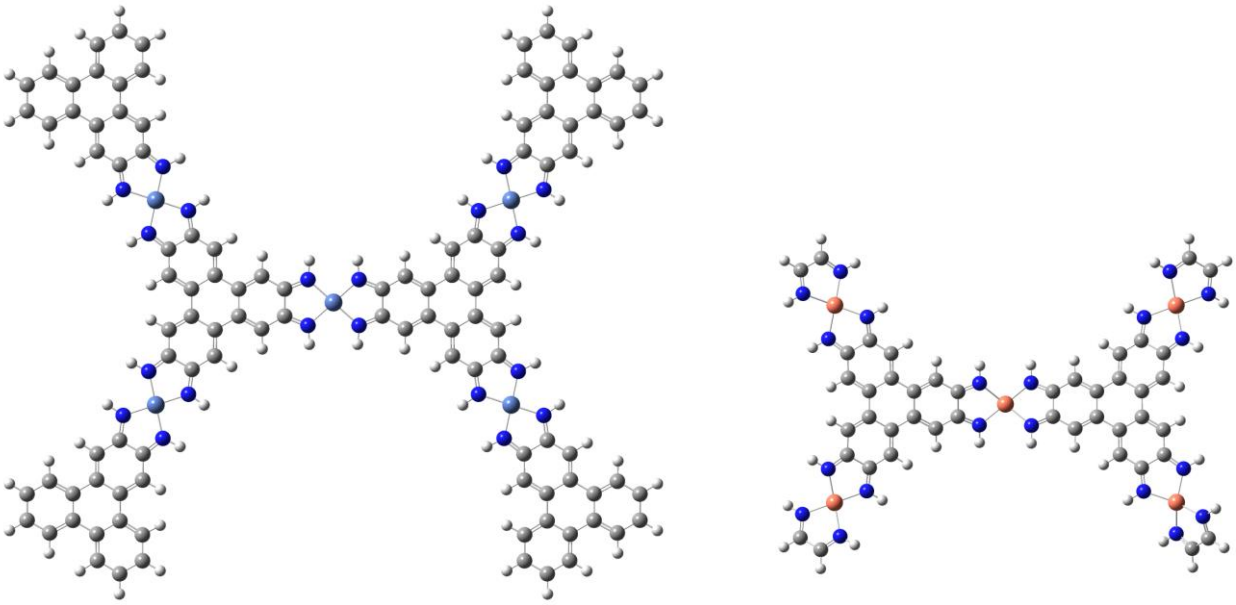
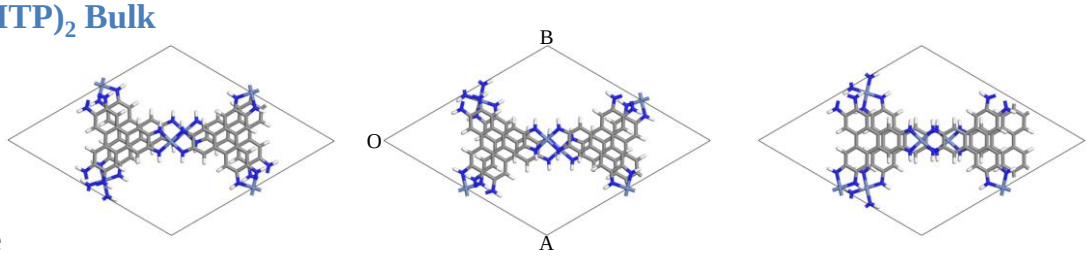


(a) Ni−HITP **(b) Cu−HITP**

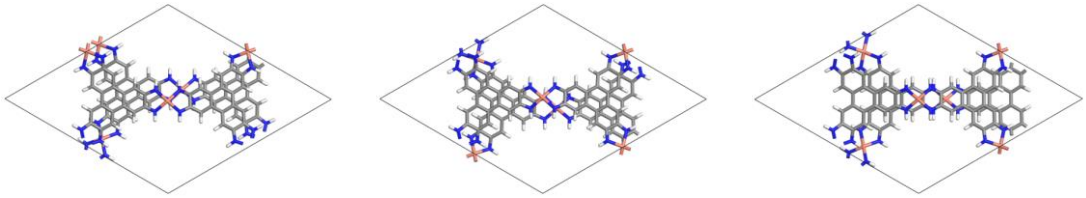
Figure S1. Optimized molecular units of (a) Ni-HITP and (b) Cu-HITP frameworks from the B3LYP/6-31G(d) calculations implemented in the Gaussian 09 software package.

(a) $Ni_3(HITP)_2$ Bulk



Relative energy (eV)	**0.00**	**2×10^{-3}**	**0.27**
***a* (Å)**	**21.850**	**21.750**	**21.813**
***b* (Å)**	**21.740**	**21.843**	**21.802**
***c* (Å)**	**6.549**	**6.547**	**6.562**
***α* (°)**	**90.0**	**90.0**	**89.9**
***β* (°)**	**90.0**	**90.0**	**89.9**
***γ* (°)**	**60.2**	**60.1**	**60.0**
	Slip along *b* axis	**Slip along *a* axis**	**Slip along *ab* axes**

(b) $Cu_3(HITP)_2$ Bulk



Relative energy (eV)	**0.00**	**0.02**	**0.56**
***a* (Å)**	**21.920**	**21.882**	**21.927**
***b* (Å)**	**21.876**	**21.931**	**21.943**
***c* (Å)**	**6.545**	**6.558**	**6.652**
***α* (°)**	**90.3**	**90.3**	**89.9**
***β* (°)**	**90.0**	**90.3**	**89.9**
***γ* (°)**	**60.2**	**60.2**	**59.8**

Figure S2. Three possible (a) $Ni_3(HITP)_2$ and (b) $Cu_3(HITP)_2$ 3D crystals with a relative shift of the second layer (~1.8 Å) along the *b* axis, *a* axis, or both *ab* axes, respectively, within the unit cell. All the crystal structures have been optimized using DFT PBE-D3 method implemented in the VASP 5.3 software package. Their relative energies and unit cell parameters are also present here.

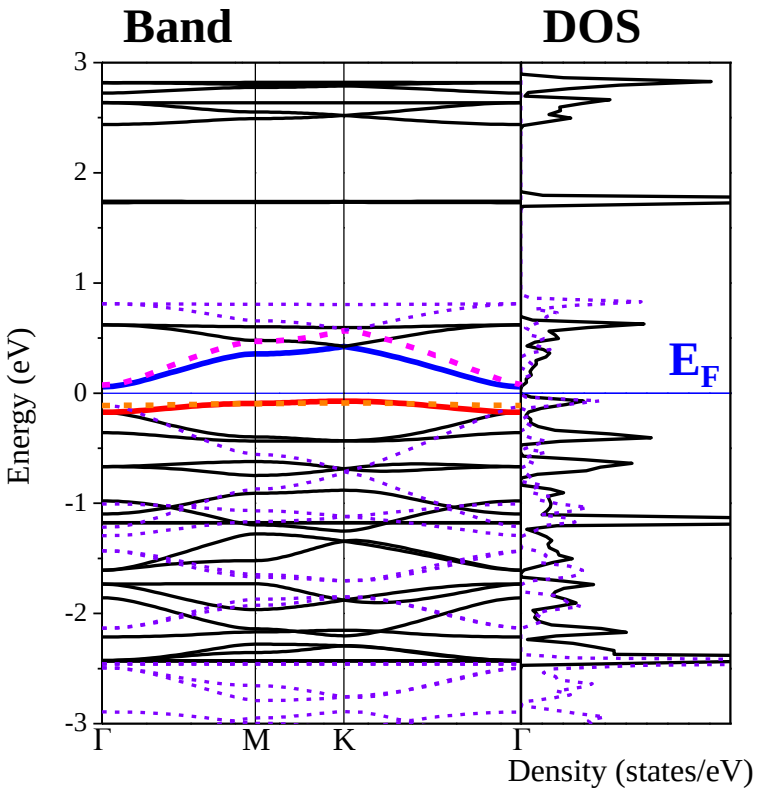
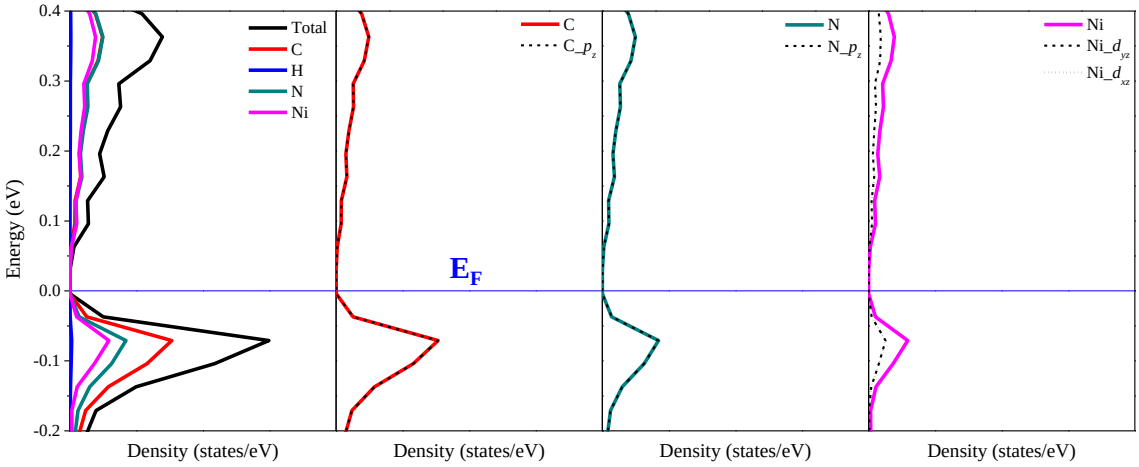


Figure S3. Comparison of computed band structures and DOS of 2D $Ni_3(HITP)_2$ sheet from PBE-D3 and HSE06 methods, both implemented in the VASP 5.3 software package. The HSE06 results are illustrated by dash lines. The Fermi level is marked by a horizontal blue line. The PBE-D3 HOVB and LUCB are highlighted in red and blue lines, respectively, whereas the HSE06 HOVB and LUCB are highlighted in orange and magenta lines, respectively.

(a) $Ni_3(HITP)_2$ Sheet



(b) $Cu_3(HITP)_2$ Sheet

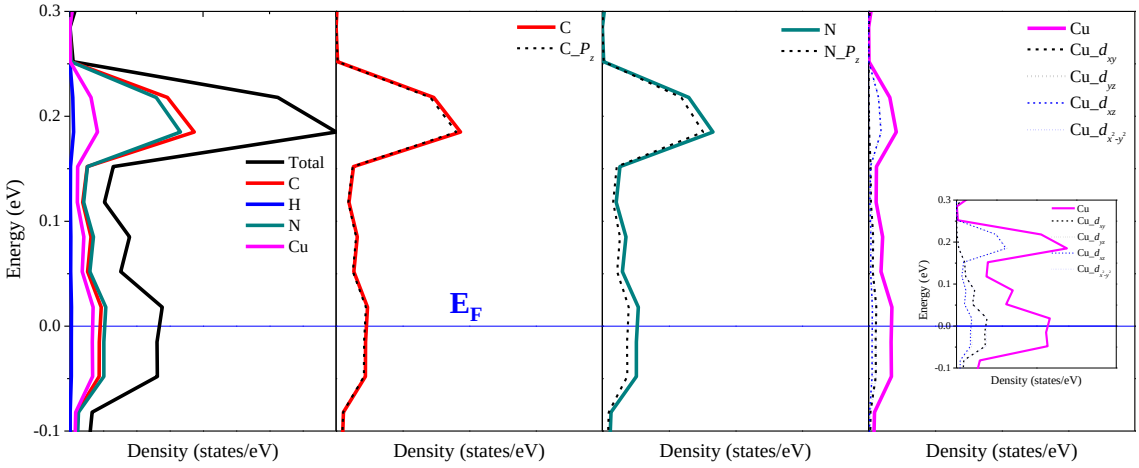


Figure S4. Computed DOS and PDOS of 2D (a) $Ni_3(HITP)_2$ and (b) $Cu_3(HITP)_2$ sheets near the Fermi level. The Fermi level is marked by the blue horizontal line. A zoom-in PDOS for the *d*-delocalized orbitals of $Cu_3(HITP)_2$ sheet is also highlighted in insets.