Electronic Supplementary Information

One-dimensional molecular chains formed by Sierpiński triangles on Au(111)†

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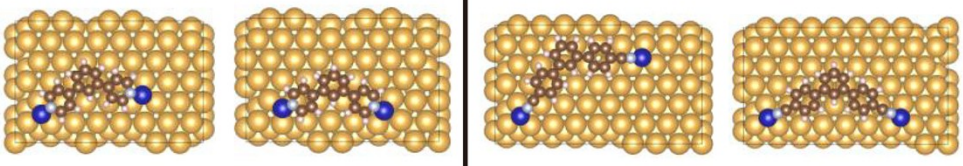
DFT calculations

DFT calculations were performed by using the 5.3.3 version of the Vienna Ab initio Simulations Package (VASP) [1,2]. The optB86 functional [3-5] was used to include the van der Waals (vdW) dispersion correction. For all calculations, an energy cut-off of 400 eV was adopted and the criterion of the force convergence of each atom was set as 0.03 eV/Å. The Brillouin zone integration was sampled using only the Γ point. The Au(111) surface is modelled by three atomic layers with the bottom two layers fixed while the atoms in topmost layer were fully relaxed.

Table 1. Adsorption energies of Co-BPyB-Co and Co-C3PC-Co motifs at representative coordinates

	Co-BPyB-Co		Co-C3PC-Co	
orientation	**(4,1)**	**(5,0)**	**(4,3)**	**(6,0)**
model				
adsorption energy ΔE_a	–9.2254 eV	–8.8410 eV	–8.3668 eV	–8.4107 eV
K value	2.4 %	6.5 %	3.7 %	2.3 %

References

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