

Supplementary Materials for
**Self-assembled nanostructures of a di-carbonitrile
molecule on copper single-crystal surfaces†**

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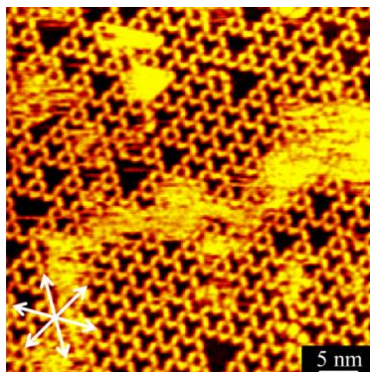


Fig. S1 STM image shows the appearance of the metal-organic coordinated nanostructures after deposition of the TPDCN molecules at room temperature on Cu(111) surface.

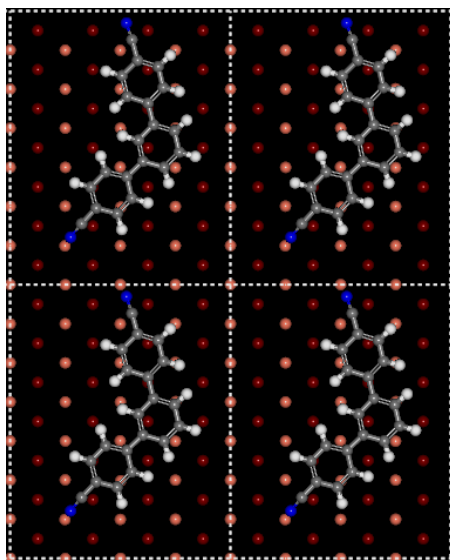


Fig. S2 The constructed supercell for the DFT calculation of the TPDCN molecule on Cu(110), which has been tested to avoid spurious interactions with neighboring cells.

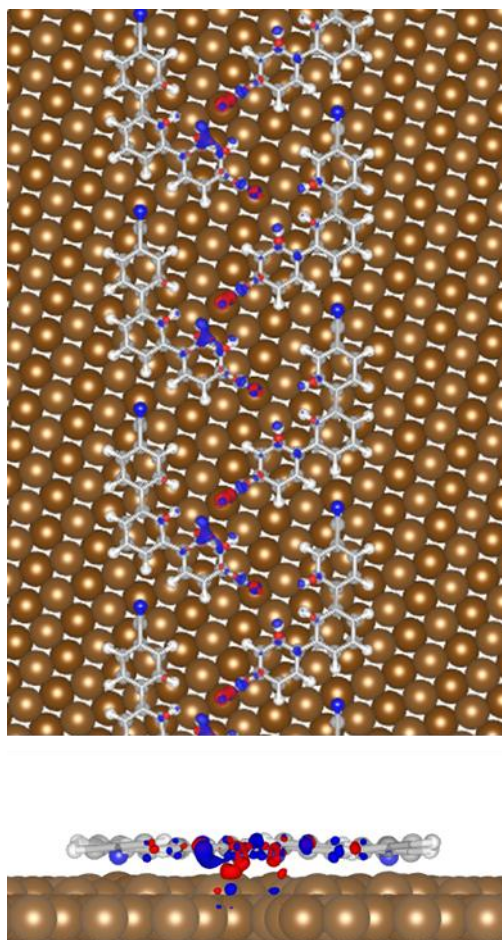


Fig. S3 The electron density difference plot of the chain on the Cu(110) surface, which is calculated at the isosurface value of $0.008 \text{ e}\text{\AA}^{-3}$. Blue and red isosurfaces indicate charge depletion and accumulation, respectively.