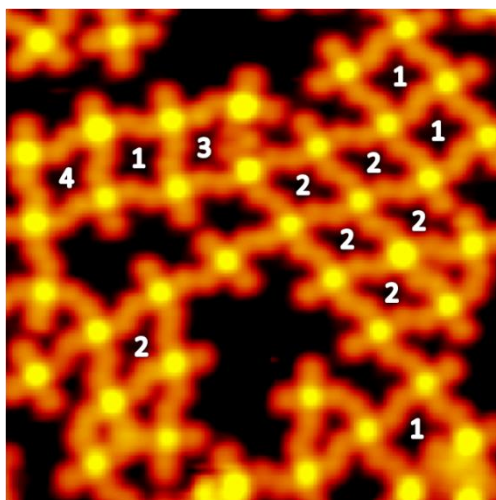


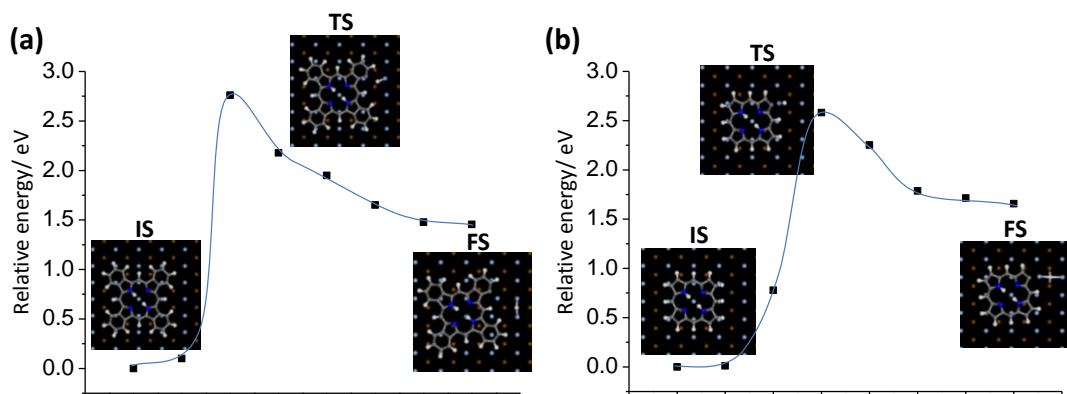
Supplementary Materials for  
**On-surface formation of two-dimensional polymer via  
direct C-H activation of metal phthalocyanine**

**Qiang Sun, Chi Zhang, Liangliang Cai, Lei Xie, Qinggang Tan and Wei Xu\***

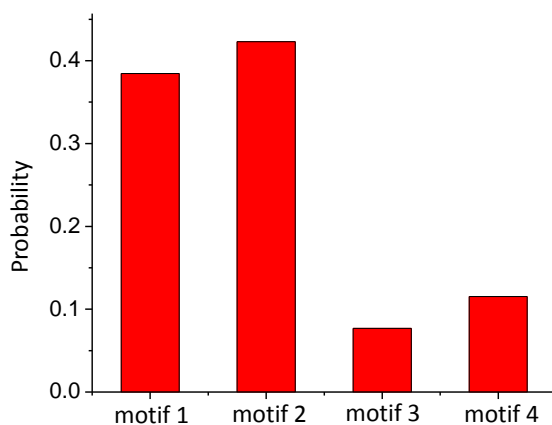
\*To whom correspondence should be addressed. E-mail: [xuwei@tongji.edu.cn](mailto:xuwei@tongji.edu.cn) (W.X.)



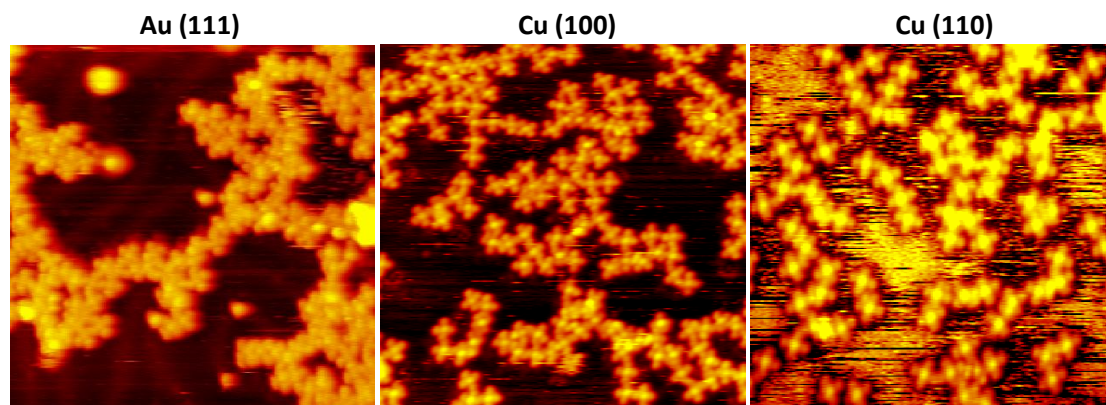
**Fig. S1.** The extended 2D nanostructure in Fig.2a is composed of the different tetramer structural motifs discussed. We have denoted the four types of motifs within the extended structure where the tetramers around the marked numbers could be identified more clearly.



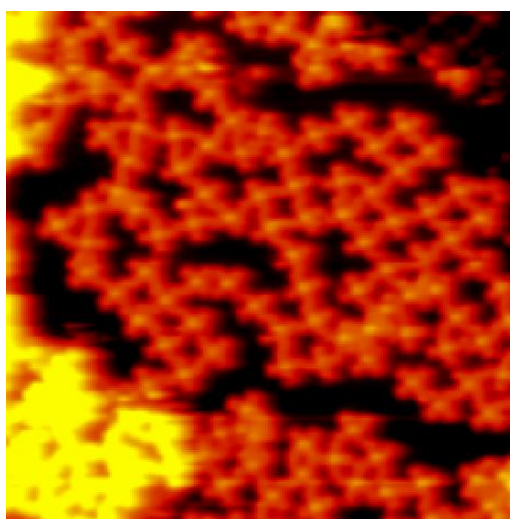
**Fig. S2.** The C-H activation barriers for (a) phthalocyanine and (b) porphyrin are determined to be about 2.7 eV and 2.6 eV, respectively. The two activation barriers are not quite different from each other, mainly because of the intrinsically similar chemical nature of the C-H bonds within these two molecules.



**Fig. S3.** The relative occurrence of the different structural motifs within the 2D polymer structures formed by CoPc on Ag(110).



**Fig. S4.** STM images showing the reaction behaviors of CoPc on Au(111) after anneal the CoPc covered sample at 680K, on Cu(100) after anneal the CoPc covered sample at 530K, and on Cu(110) after anneal the CoPc covered sample at 500K, respectively.



**Fig. S5.** STM image after annealing the CoPc covered Ag(110) surface at ~750K.