Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Transformation of the coordination nanostructures of 4,4',4''-(1,3,5-Triazine-2,4,6-triyl) tribenzoic acid molecule on HOPG triggered by the change in the concentration of metal ions

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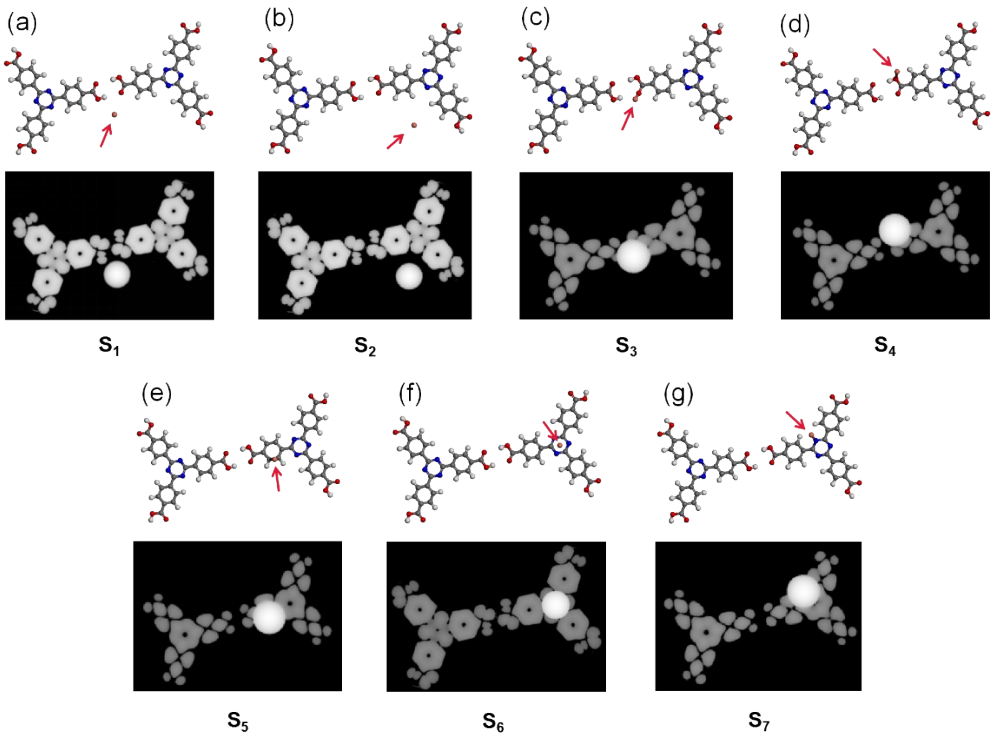
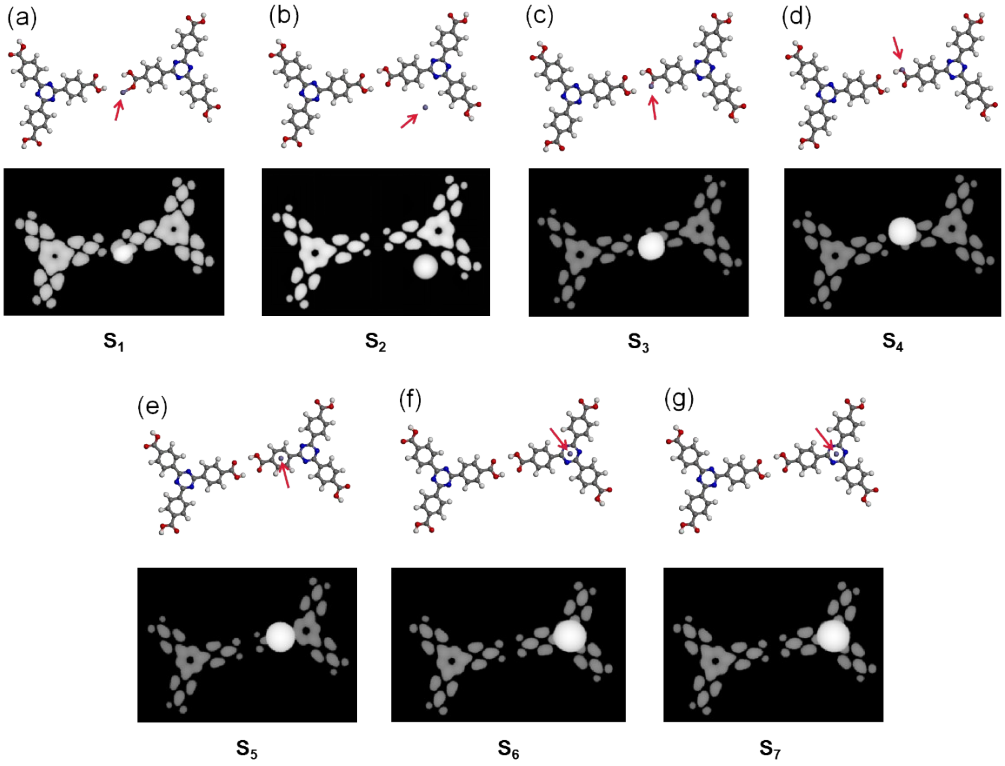


Supplementary Figure 1. (a)-(g) The optimized structure models and STM simulation images of Cu^{2+} adsorbed on seven potential sites (S_1-S_7) of TATB dimer, respectively. The red arrow in the figure indicates the position of Cu^{2+}.



Supplementary Figure 2. (a)-(g) The optimized structure models and STM simulation images of Fe^{3+} adsorbed on seven potential sites (S_1-S_7) of TATB dimer, respectively. The red arrow in the figure indicates the position of Fe^{3+}.

DFT calculations were performed on the structural models of the seven adsorption sites of Cu^{2+}/Fe^{3+} on the TATB dimer, respectively. The optimized structure models and STM simulation images as shown in supplementary Figure 1 and 2. For the proposed structural model, Cu^{2+}/Fe^{3+} is at the same height as the TATB molecular plane at the S_1 and S_2 sites, and is about 2.8 Å higher than the TATB molecular plane at the S_3-S_7 sites. As shown in supplementary Figure 2f and 2g, it is identical with the optimized adsorption site and the STM simulation image of Fe^{3+} adsorbed on TATB dimer at S_6 or S_7 site.