Supplementary Information for

"Electronic and magnetic properties of CoPc and FePc molecules on graphene: substrate, defect and hydrogen adsorption effects"

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S1. Active orbital of free FePc calculated by CASSCF

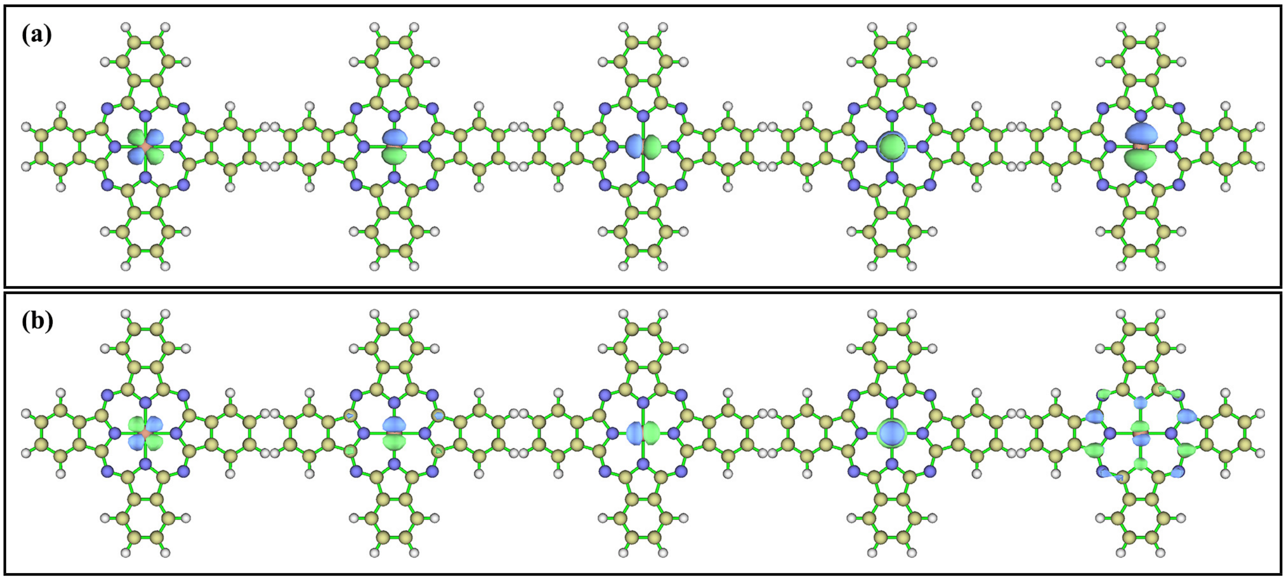

Figure S1. The upper and lower panels show the five active orbital of free FePc include predominant d atomic orbital character as calculated by the CASSCF method including (a) six triplets and one singlet or (b) three quintets, six triplets and one singlet states. Obviously, the last active orbital in (b) contains less d atomic orbital character than others. The default isovalue is 0.05 a.u. The molecular orbitals are rendered by Multiwfn.[1]

S2. PDOS of the $3d$ orbitals in the Fe ion in FePc/G

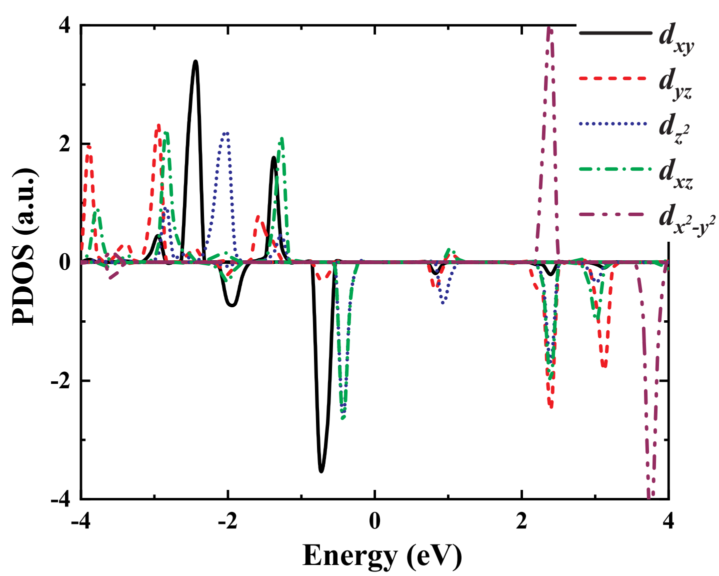

Figure S2. The spin-polarized PDOS of five $3d$ orbitals of the Fe ion in the FePc/G composite.

S3. Spin density of the H-FePc/G/Au(111) composite

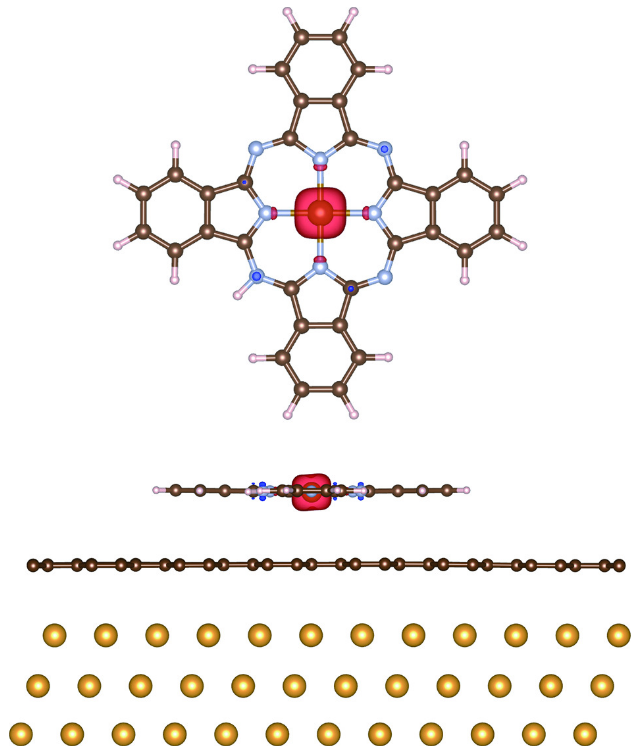

Figure S3. The spin density distribution in the H-FePc/G/Au(1111) composite. Red (blue) symbols correspond to the majority (minority) spin. The isovalue for the spin density is 0.01 Å^{-3}.

S4. Kondo temperature of the SU(4) symmetrical Anderson model

The closed analytical expression for the Kondo temperature of the SU(4) symmetrical Anderson model derived in Ref. 2 via a path integral approach is

$$k_B T_{\mathrm{K,SU(4)}} = U_1 f\left(\frac{\epsilon_1}{U_1}\right)\left[\frac{-2J_1U_1}{\pi\epsilon_1(\epsilon_1+U_1)}\right]^{\frac{1}{4}} \exp\left[\frac{\pi\epsilon_1(\epsilon_1+U_1)}{2J_1U_1}\right]$$

with

$$f(x) = \left[-x(x+1)^3\right]^{\frac{1}{4}} \exp\left[g(x)\right]$$

and

$$g(x) = \frac{3x-2}{4(x+2)} - \frac{x^2(x^2+3x+3)}{2(x+2)^2} \ln\left(\frac{2x+3}{x+1}\right)$$

REFERENCES

[1] T. Lu and F. Chen, J. Comput. Chem. **33**, 580 (2012).

[2] M. Filippone, C. P. Moca, G. Zaránd, and C. Mora, Phys. Rev. B **90**, 121406 (2014).