Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

"Unravelling the robustness of magnetic anisotropy of a nickelocene molecule in different environments: A first-principles-based study"

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S1. DFT-D3 results for Nc/Cu(100)

Table S1. Relative total energies, blinding energies (in units of eV) and the total magnetic moments (in units of μ_B) of Nc along with the contributions from the Ni atom for three different Nc/Cu(100) adsorption configurations calculated by the DFT-D3 method.

Nc/Cu(100)	Top	Bridge	Hollow
Energy	0.39	0.31	0.00
Blinding Energy	-1.07	-1.15	-1.46
Total magnetism	0.00	0.00	2.24
Ni magnetism	0.01	0.00	0.98

In the manuscript, we adopted the DFT-D2 method to verify our theoretical simulation reliable compared with that of the original research paper.[1] Here, we also perform additional calculations with the DFT-D3 method, and the related results are listed in Table S1. As can be found in Table S1, the DFT-D3 calculations have no significant difference from that with the DFT-D2 method. For example, the favorite adsorption configuration is still the hollow site, and the corresponding magnetic moment of Nc in the composite is 2.24 μ_B, almost the same with that by the DFT-D2 method.

S2. Electronic structures of three configurations of Nc/Cu(100)

Table S2. Relative total energies and magnetic moments for different Nc/Cu(100) configurations.

Nc/Cu(100)	Energy (eV)	Binding Energy (eV)	Magnetic moment (μ_B)
Top	0.26	-1.15	0.00
Bridge	0.03	-1.38	1.12
Hollow	0.00	-1.41	2.25

Table S3. The amounts of the transferred net electrons from Nc to Cu and on the Ni center when Nc adsorbed on different sites on Cu(100) by the the Bader charge analysis.

Nc/Cu(100)	Top	Bridge	Hollow
from Nc to Cu	0.22	0.13	0.06
on the Ni center	0.076	0.039	0.023

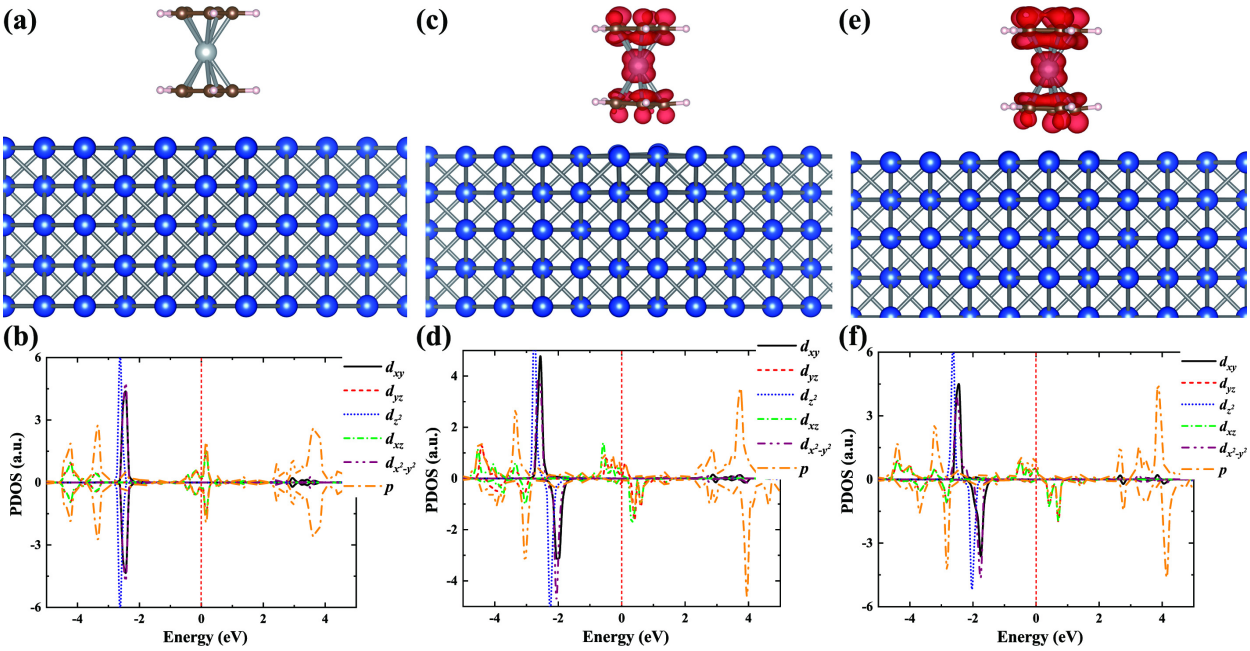

Figure S1. The three panels (left to right) show the spin density distribution and spin-polarized PDOS of Nc onto five $3d$ orbitals of the Ni atom and all p carbon orbitals in the top, bridge and hollow adsorption configurations of Nc/Cu(100), respectively. Red (blue) symbols correspond to the majority (minority) spin in Figs. S1(a), (c) and (e). The isovalue for the spin density is $0.0025\,\mathrm{Bohr}^{-3}$. The red vertical dash lines in Figs. S1(b), (d) and (f) indicate the Fermi energy E_F that is set to zero.

REFERENCES

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