Electronic Supplementary Information

Robust Sierpiński triangle fractals on symmetry-mismatched Ag(100)

Xue Zhang,[a§] Na Li,[a§] Liwei Liu,[a] Gaochen Gu,[a] Chao Li,[a] Hao Tang,[b] Lianmao Peng,[a] Shimin Hou[ac] and Yongfeng Wang*[ac]

[a.] *Key Laboratory for the Physics and Chemistry of Nanodevices, Department of Electronics, Peking University, Beijing 100871, China.*

[b.] *CEMES-CNRS, Boîte Postale 94347, 31055 Toulouse, France.*

[c.] *Beida Information Research (BIR), Tianjin 300457, China.*

**Corresponding author. E-mail: yongfengwang@pku.edu.cn*

[§]*These authors contributed equally.*

Method of DFT calculations

In these calculations, the core electrons were described by the pseudopotentials constructed according to the projector augmented wave (PAW) method.[1] The exchange-correlation energy was calculated with the Perdew-Burke-Ernzehof[2,3] (PBE) functional in the Generalized Gradient Approximation (GGA). $5s^14d^{10}$, $2s^22p^2$, $2s^22p^4$, $1s^1$ and $4s^13d^7$ valence electrons were used respectively for Ag, C, O, H and Fe. The lattice parameter of bulk Ag was optimized to 4.162 Å (4.085 Å for the experimental value) with a kinetic energy cutoff of 500 eV and a 13×13×13 Monkhorst-Pack mesh[4] for the sampling of the Brillouin zone. The DFT-D2 method[5] was used for molecule on surface calculations in order to take into account the van der Waals (vdW) dispersive correction. As this correction could introduce no desired modification of surface properties,[6] it was applied only for molecule-surface, molecule-molecule and intra-molecule interactions. The $Fe(H3PH)_3$ complex is adsorbed with the Fe located at the hollow site of Ag(100) surface. The average height of this complex is 2.9 Å above the Ag surface, while the Fe is slightly lower (2.47 Å). Upon adsorption, 0.58 electron was transferred from the substrate to the complex. The magnetic moment of Fe is 3.48 m_B. The Ag(100)

surface was modelled by a slab of 336 atoms composed by 4 atomic layers. During the geometric relaxation, atoms in the bottom 2 layers were kept fixed and the electronic self-consistent field was converged within 1×10^{-6} eV, while as the forces on each atom were smaller than 0.02 eV/Å for the geometric optimization. The super-cell containing molecule-slab has a dimension of 24.97 Å × 29.13 Å × 18.32 Å. Only Γ point was used for the Brillouin zone sampling.

References

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