Supplementary material of

The shielding effects of C_{60} cage on the magnetic moments of Transition Metal atoms inside corner holes of Si(111)-(7×7)

Xiji Shao,[a,b,c] Lin Li,[d] Xingqiang Shi,[b] Yaping Ma,[e] Xuefeng Wu,[b] Kedong Wang*[b,c]

[a.] *Harbin Institute of Technology, Harbin 150080, China.*

[b.] *Department of Physics, Southern University of Science and Technology, Shenzhen 518055, China. E-mail: wangkd@sustech.edu.cn*

[c.] *Shenzhen Key Laboratory of Quantum Science and Engineering, SUSTech, Shenzhen 518055, China.*

[d.] *College of Physics and Electronic Engineering, and Center for Computational Sciences, Sichuan Normal University, Chengdu 610068, China*

[e.] *SZU-NUS Collaborative Innovation Center for Optoelectronic Science & Technology, Shenzhen University, Shenzhen 518060,China*

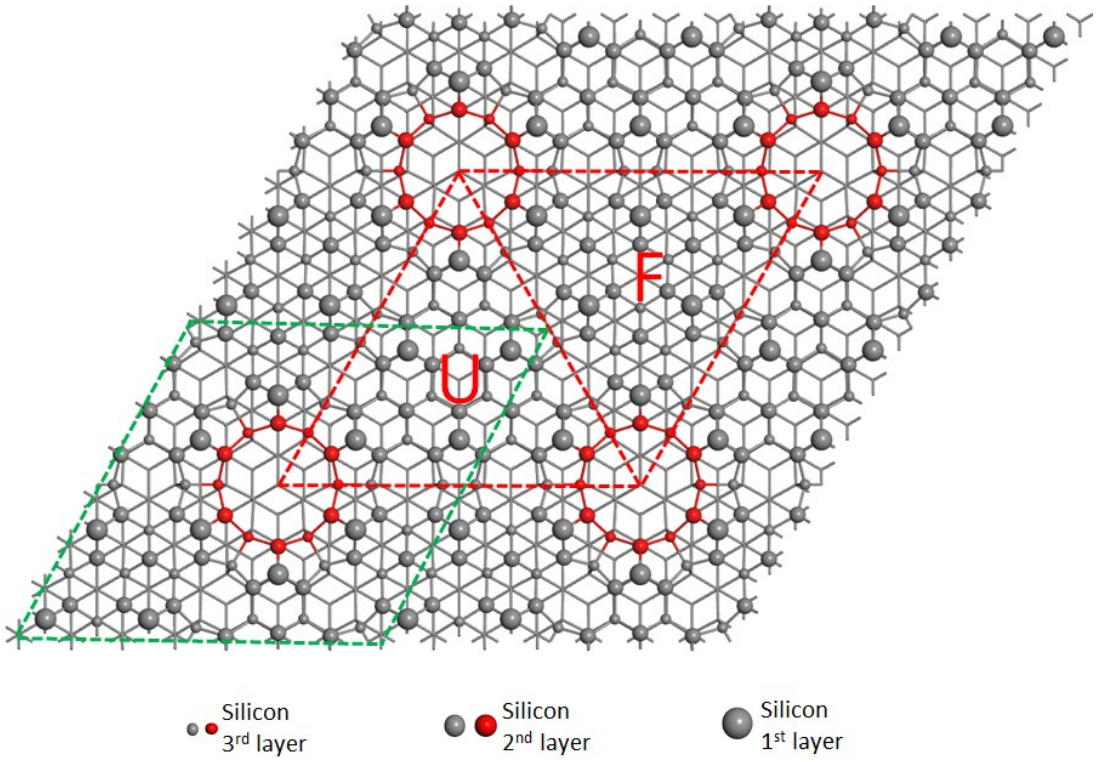

Figure S0. The red dashed lines indicate a usually used unit cell of Si(111)-7x7 surface. The letters “F” and “U” show the faulted and unfaulted half unit cells, respectively. While the unit cell we used in the current paper is the one shown with the green lines.

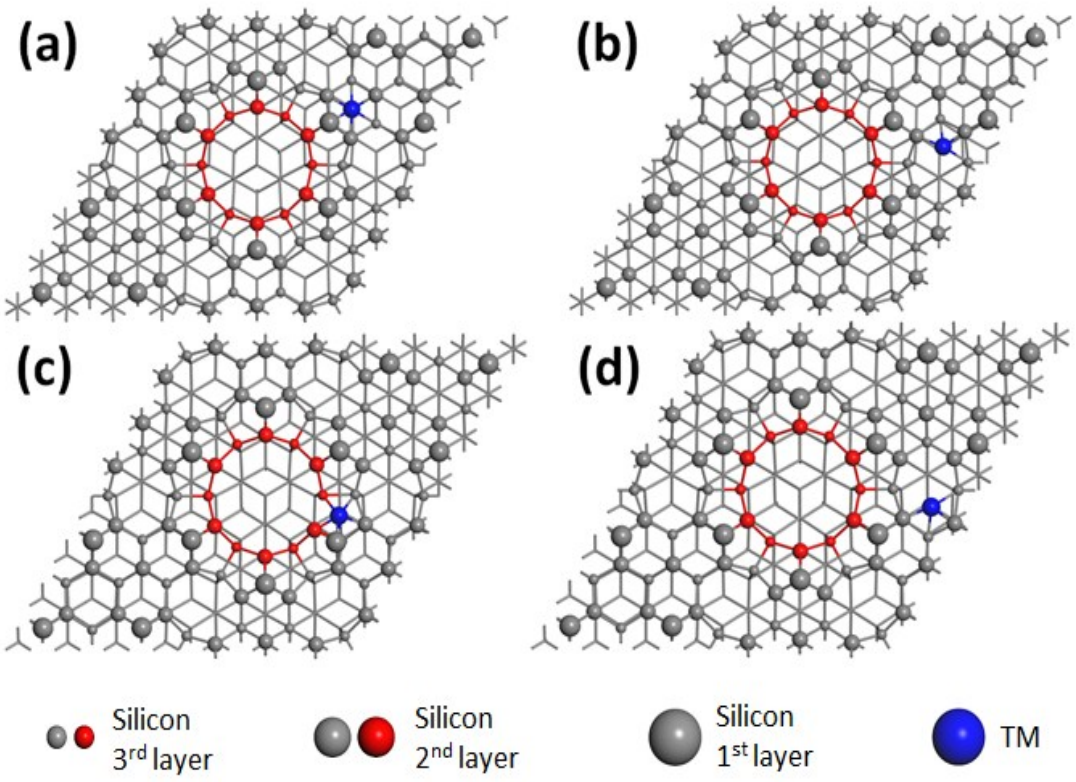

Figure S1. Top view of TM atoms adsorb on various sites of the Si(111)-(7×7) outside the corner hole. The corresponding adsorption energies are listed in table S1.

Table S1. The adsorption energies for TMs adsorb on the surface of Si(111)-(7×7) at various sites (eV). The data show that the corner hole is the most stable adsorption site for all the three TM atoms.

TM atom\Sites	Fig. S1(a)	Fig. S1(b)	Fig. S1(c)	Fig. S1(d)	**Hole**
Fe	3.71	2.76	3.43	2.76	**3.78**
Co	4.22	3.38	4.24	3.38	**4.58**
Ni	4.26	3.57	4.07	3.57	**4.36**

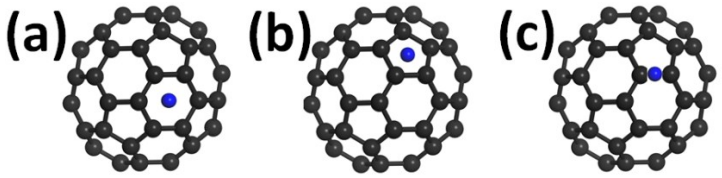

Figure S2. Possible adsorption sites of TM atoms inside a C_{60} molecule that considered in our calculations. (a) near the center of a six-membered ring, (b) near the center of a five-membered ring, and (c) near the center of a C-C bridge.

Table S2. The adsorption energies for TMs adsorb inside the C_{60} (eV). The most stable sites for all the three TM atoms are located close to the center of a carbon six-membered ring.

TM atoms\Sites	Near the center of a six-membered ring	Near the center of a five-membered ring	Bridge
Fe	0.62	0.52	Not stable
Co	1.11	0.75	Not stable
Ni	0.95	0.54	Not stable

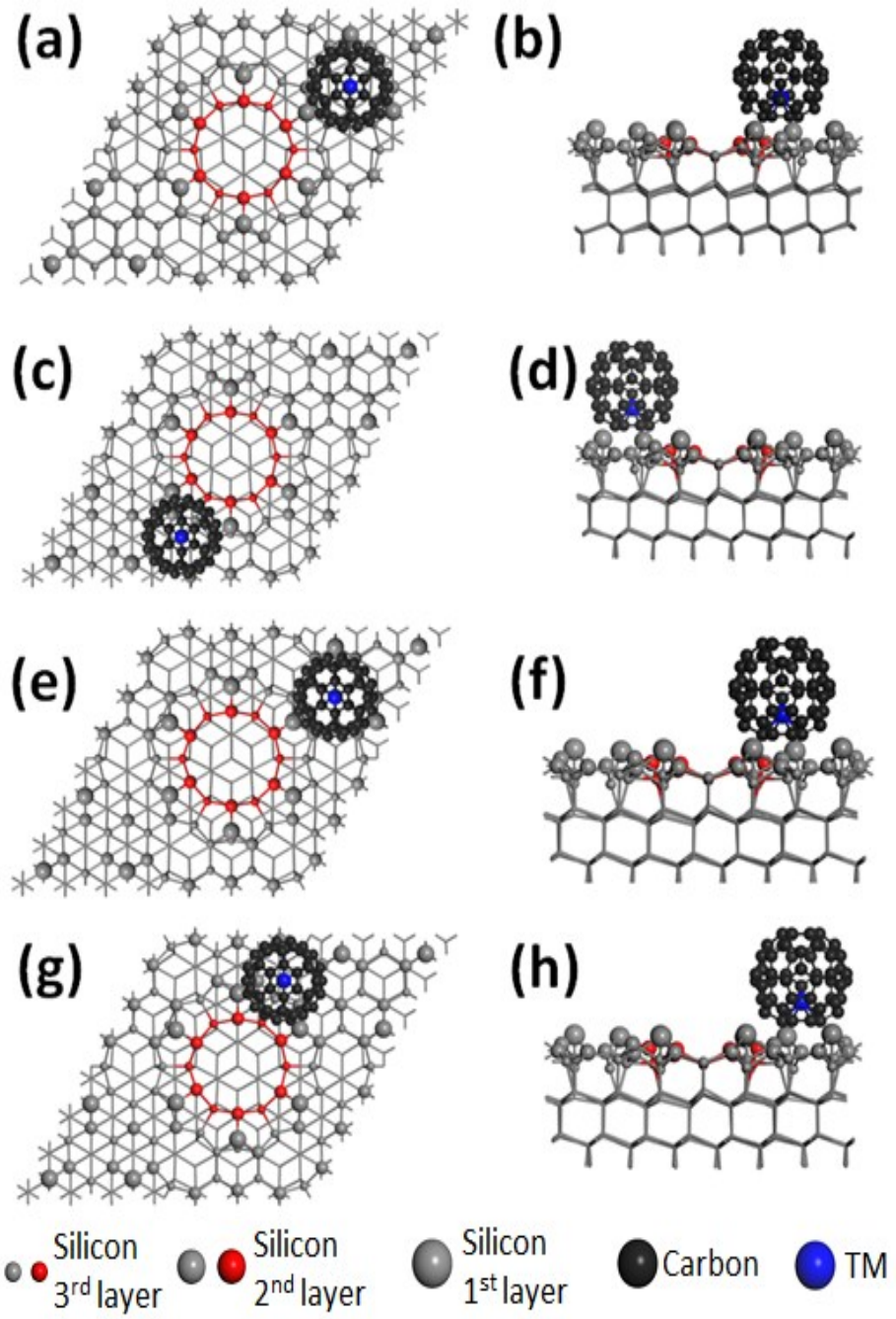

Figure S3. (a), (c), (e), (g)Top view and, and (b), (d), (f), (h) side view of TM@C_{60} adsorb on the surface of the Si(111)-(7×7) outside the corner hole.

Table S3. The adsorption energies of TM@C60 adsorb on different sites of the surface of Si(111)-(7×7) shown in figure S3 as well as the corner hole site (eV). The corner hole site is the most stable site for all the TM@C_{60}.

systems	(a)(b)	(c)(d)	(e)(f)	(g)(h)	**hole**
Fe	0.81	0.48	0.80	0.46	**0.92**
Co	0.81	0.71	0.81	0.70	**1.61**
Ni	0.75	0.38	0.76	0.38	**0.43**

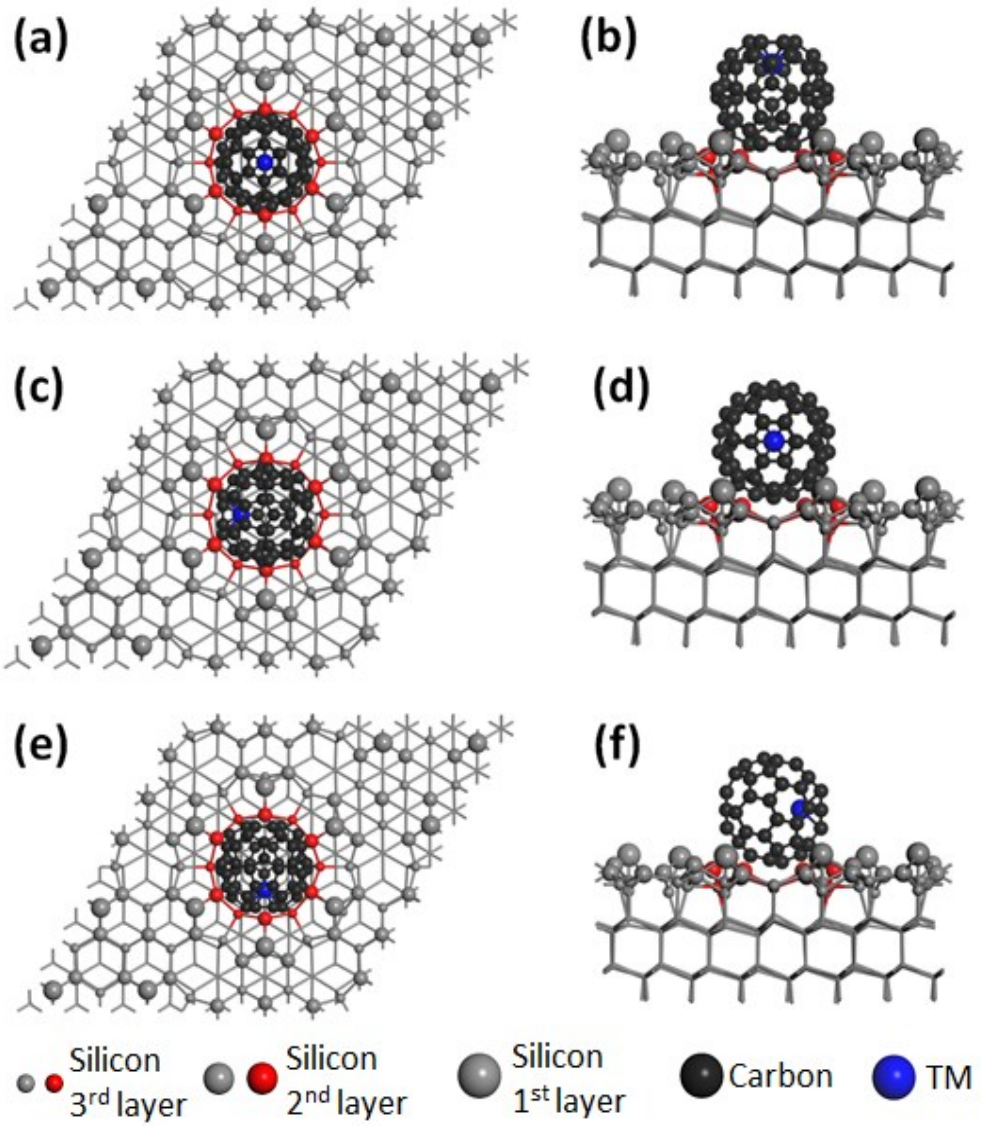

Figure S4. (a), (c) and (e) top view, and (b), (d), (f) side view of TM@C_{60} adsorb inside the corner hole of Si(111)-(7×7) with different orientations.

Table S4. The adsorption energy for TM@C_{60} adsorb inside the corner hole of Si(111)-(7×7) with various orientations as well as the one shown in the main text (eV). The orientation shown in the main text has the highest adsorption energy for all the TM atoms.

systems	(a)(b)	(c)(d)	(e)(f)	**hole**
Fe	0.74	0.32	0.38	**0.92**
Co	0.91	0.64	0.31	**1.61**
Ni	0.81	0.53	0.46	**1.43**

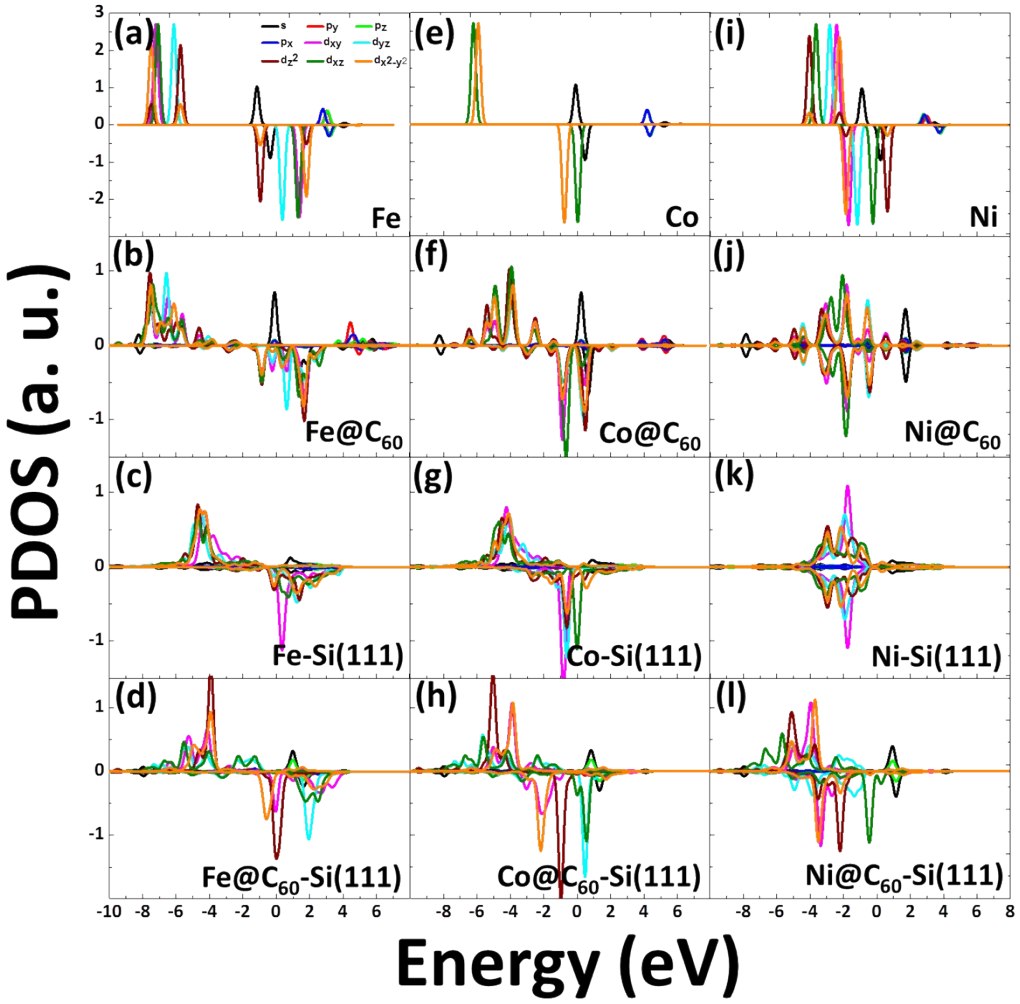

Figure S5. The PDOS of TM atoms in different configurations.