Supporting information

for

Electronic and magnetic properties of Au-doped diamond surface by first-principles calculation

Wei Cheng, Cong Li, Tianyi Wang, Shaoheng Cheng, Nan Gao*, and Hongdong Li*

State Key Lab of Superhard Materials, College of Physics, Jilin University,

Changchun 130012, China

*Corresponding Authors

E-mail address: gaon@jlu.edu.cn, hdli@jlu.edu.cn.

Table S1 Adsorption energy, areal electron density and magnetic moment of Au atom at different sites for diamond (100), (111) and (100) surfaces.

orientation	position	adsorption energy (eV)	areal electron density (cm^{-2})	magnetic moment (μ_B)
100	P1	-0.636	1.97×10^{13}	0.902
	P2	-0.583	1.67×10^{13}	0.949
	P3	-0.511	1.32×10^{13}	0.911
	P4	-0.496	1.34×10^{13}	0.927
	P5	-0.635	1.88×10^{13}	0.925
111	P1	-0.673	6.34×10^{13}	0.994
110	P1	-0.656	3.14×10^{13}	0.941

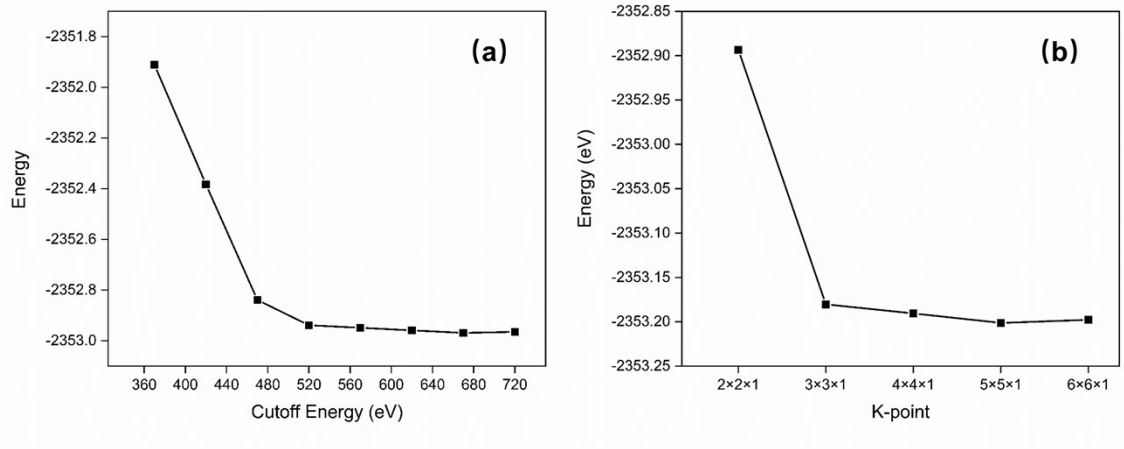

Fig. S1. Convergence tests of diamond (100) surface with the variation of (a) cut-off energy and (b) k-point.

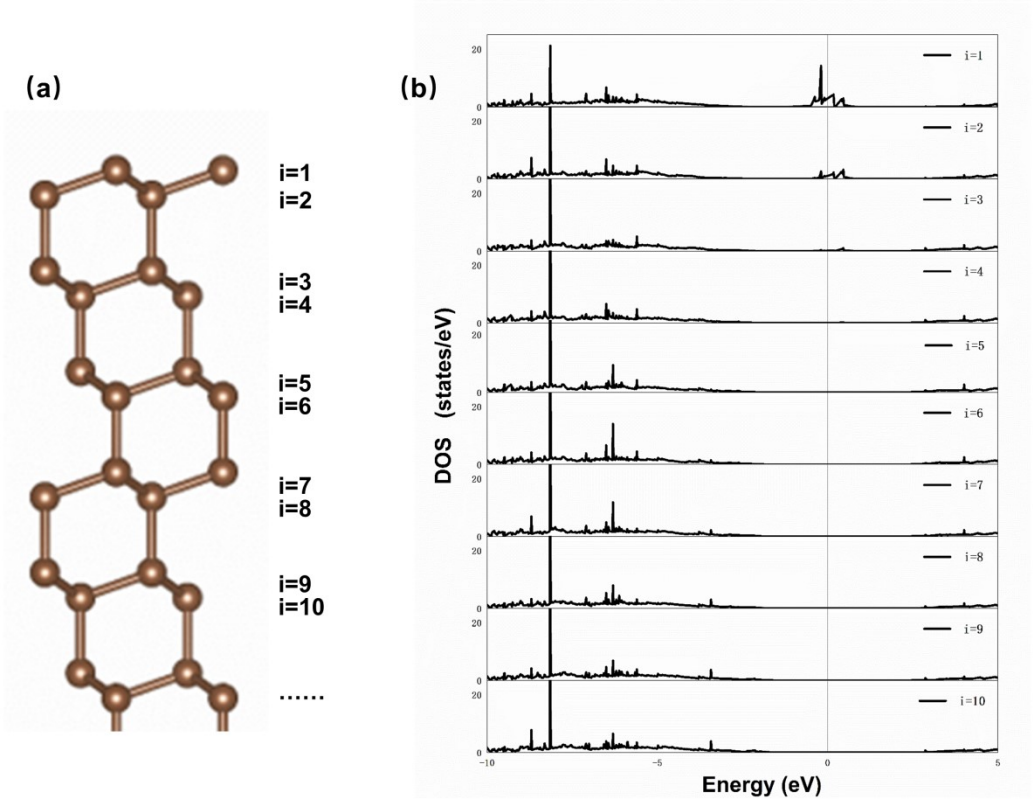

Fig. S2. (a) Structural model and (b) DOS of diamond (111) surface with the variation of the layers.

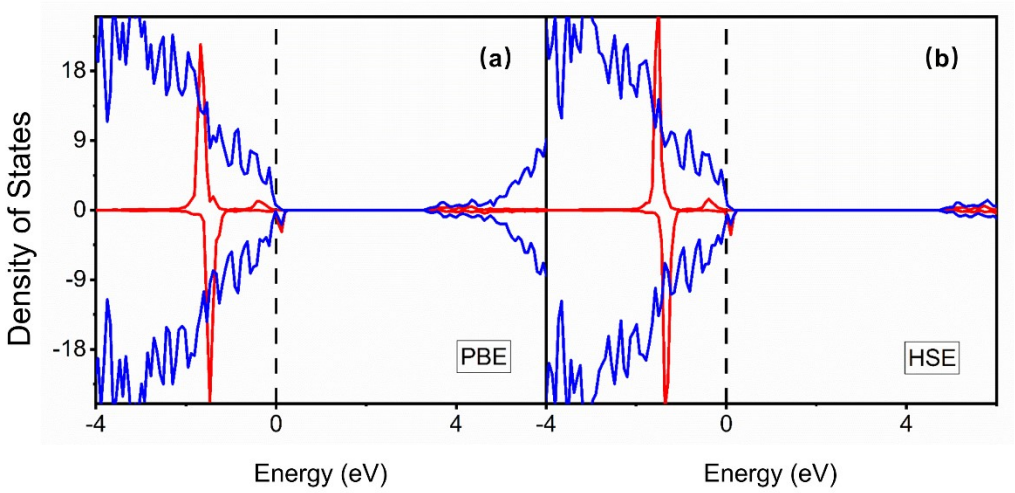

Fig. S3. DOS for Au-doped diamond (100) surface with the functionals of (a) PBE and (b) HSE.

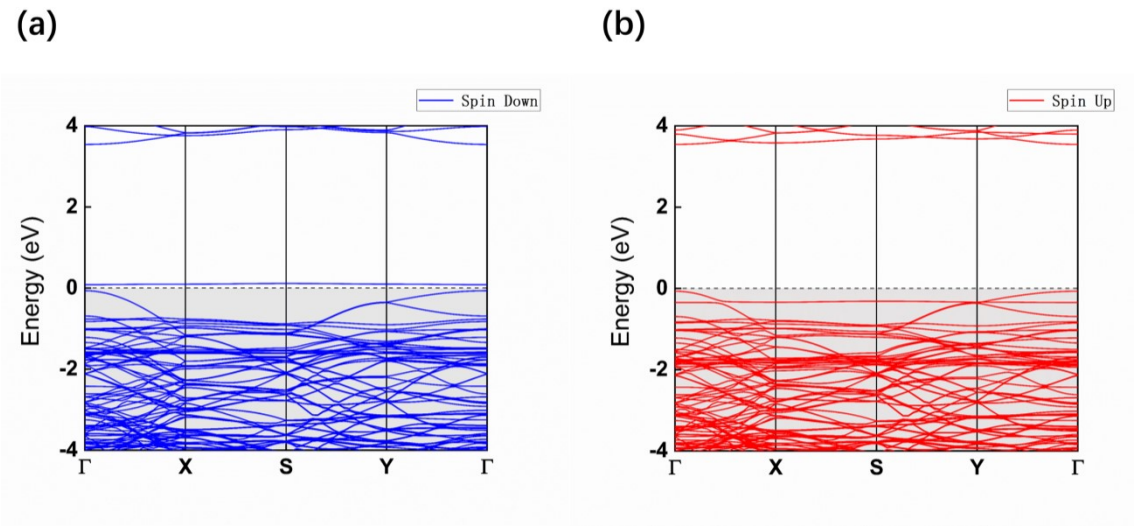

Fig. S4. (a) Spin-down and (b) spin-up band structures of Au-doped diamond (100) surface.

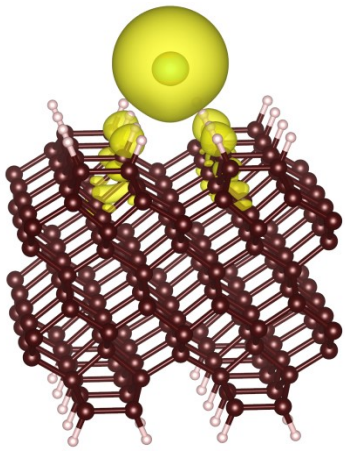

Fig. S5. Spin density distribution of diamond (100) surface doped with Au. The isosurface value is 0.0007 e $Å^{-3}$.

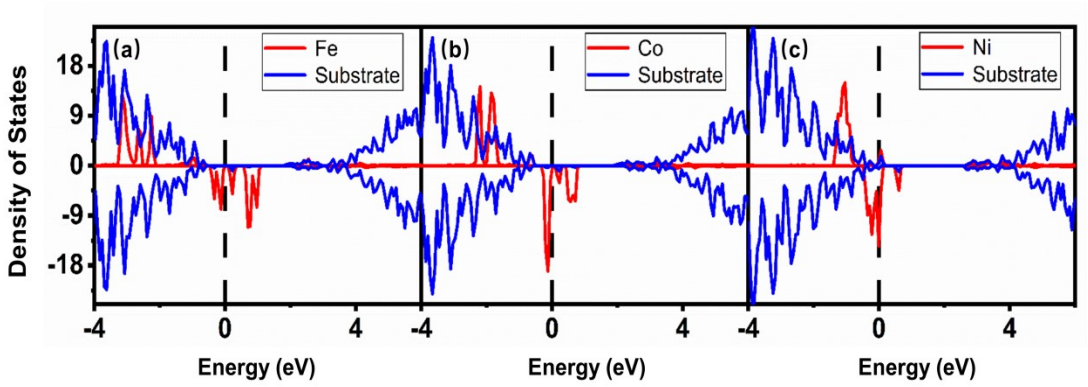

Fig. S6. DOS of (a) Fe, (b) Co, and (c) Ni doped diamond (111) surfaces. The Fermi level is set to zero.

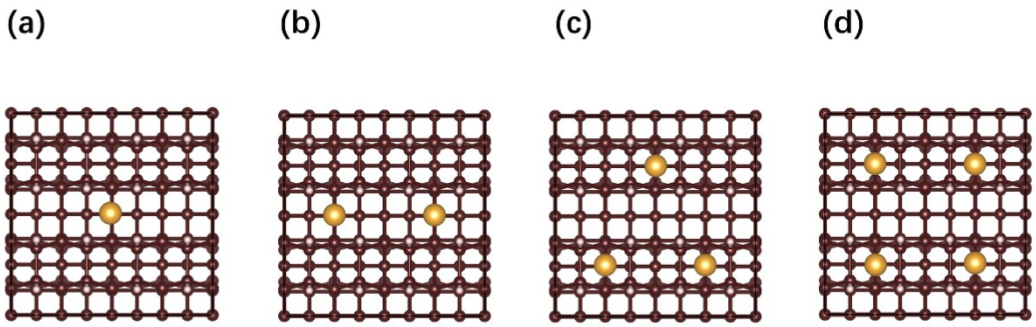

Fig. S7. Structures of Au-doped diamond for different doping rate at (a) 0.125 ML, (b) 0.25 ML, (c) 0.375 ML, and (d) 0.5 ML.

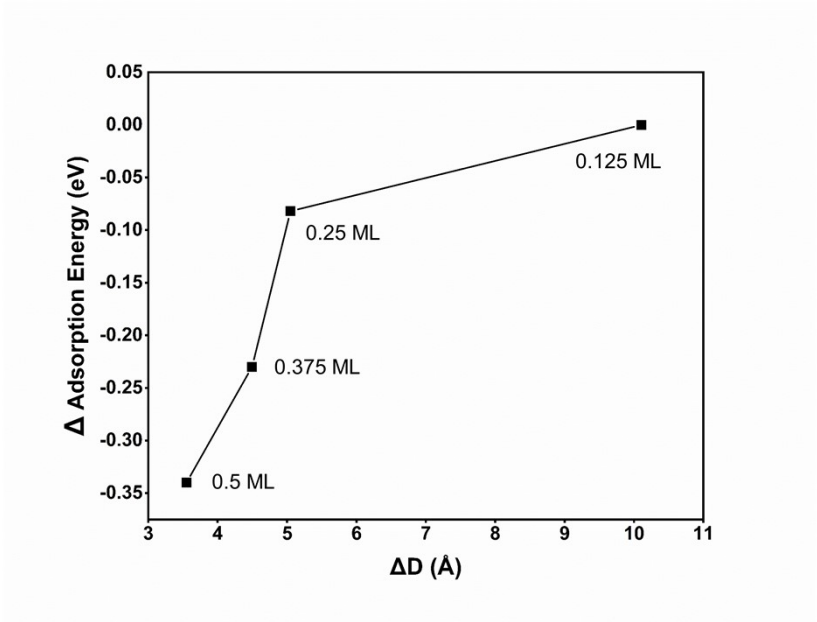

Fig. S8. The amount of change in adsorption energy of diamond (100) surface as a function of distance between two nearest neighboring Au atoms on diamond surface. The magnitude of the adsorption energy for a single Au at a coverage of 0.125 ML was used as a benchmark to obtain the corresponding change in adsorption energy.

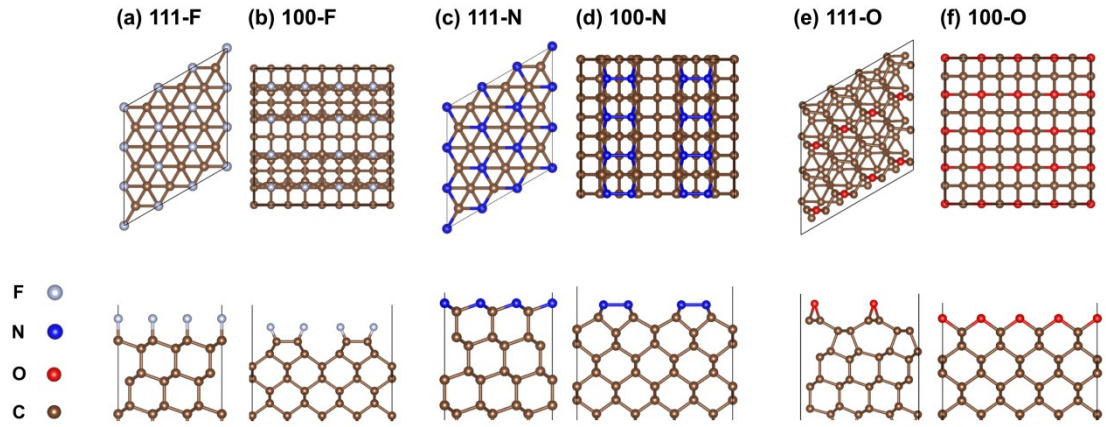

Fig. S9. Side and top views of diamond surfaces with (a) 111-F, (b) 100-F, (c) 111-N, (d) 100-N, (e) 111-O, and (f) 100-O.