Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Supplementary information

Adjustable electronic performances and redox ability of g–C_3N_4 monolayer by absorbing nonmetal solute ions: A first principles study

S. Lu[1], Z. W. Chen[2], C. Li[1]*, H. H. Li[1], Y. F. Zhao[1], Y. Y. Gong[1], L. Y. Niu[1], X. J. Liu[1] T. Wang[3] and C. Q. Sun[1,4]

[1] Center for Coordination Bond Engineering, College of Materials Science and Engineering, China Jiliang University, Hangzhou 310018, China

[2] Key Laboratory of Automobile Materials, Ministry of Education, Department of Materials Science and Engineering, Jilin University, Changchun 130022, China

[3] College of Electrical Engineering, Zhejiang University, Hangzhou 310027, China

[4] School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore 639798

*E-mail: canli1983@gmail.com

Table S1. The wavelength of optical absorption edges λ_{edge} with unit nm. The integral area of optical absorption curves in ultraviolet (S_{UV}) and visible light (S_V) regions with uniform unit.

system	λ_{edge}		S_{UV}		S_V	
	2×2	3×3	2×2	3×3	2×2	3×3
pristine	455	461	626	558	216	205
H	462	455	619	601	152	129
B	449	447	608	578	237	205
C	449	445	610	585	200	191
Si	446	444	714	680	230	195
N	442	445	578	558	224	191
P	468	460	629	587	224	140
As	455	448	630	606	216	181
O	453	450	613	594	264	246
S	454	452	644	628	227	202
Se	458	454	635	609	199	162
Te	452	454	652	615	161	175
F	448	455	672	651	153	180
Cl	450	448	694	671	143	113
Br	458	451	701	682	143	110
I	453	449	702	680	144	117

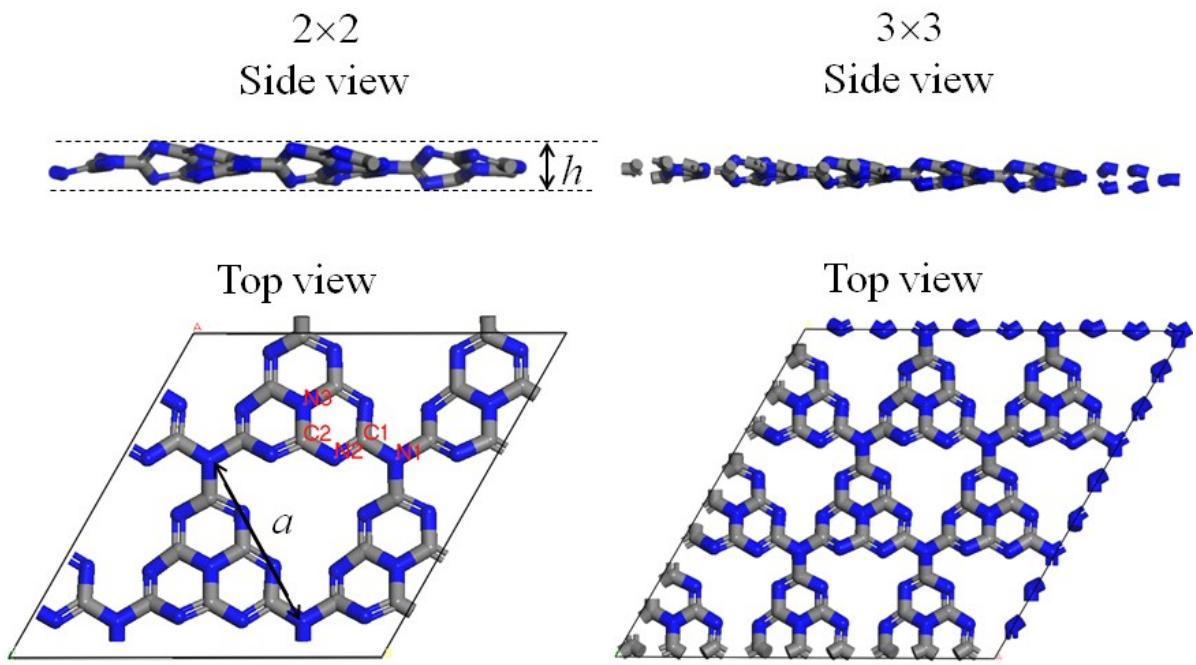

Figure S1. (Color online) Schematic structures of the 2×2 and 3×3 supercell g–C_3N_4 monolayer, where the gray and blue spheres denote the C and N atoms.

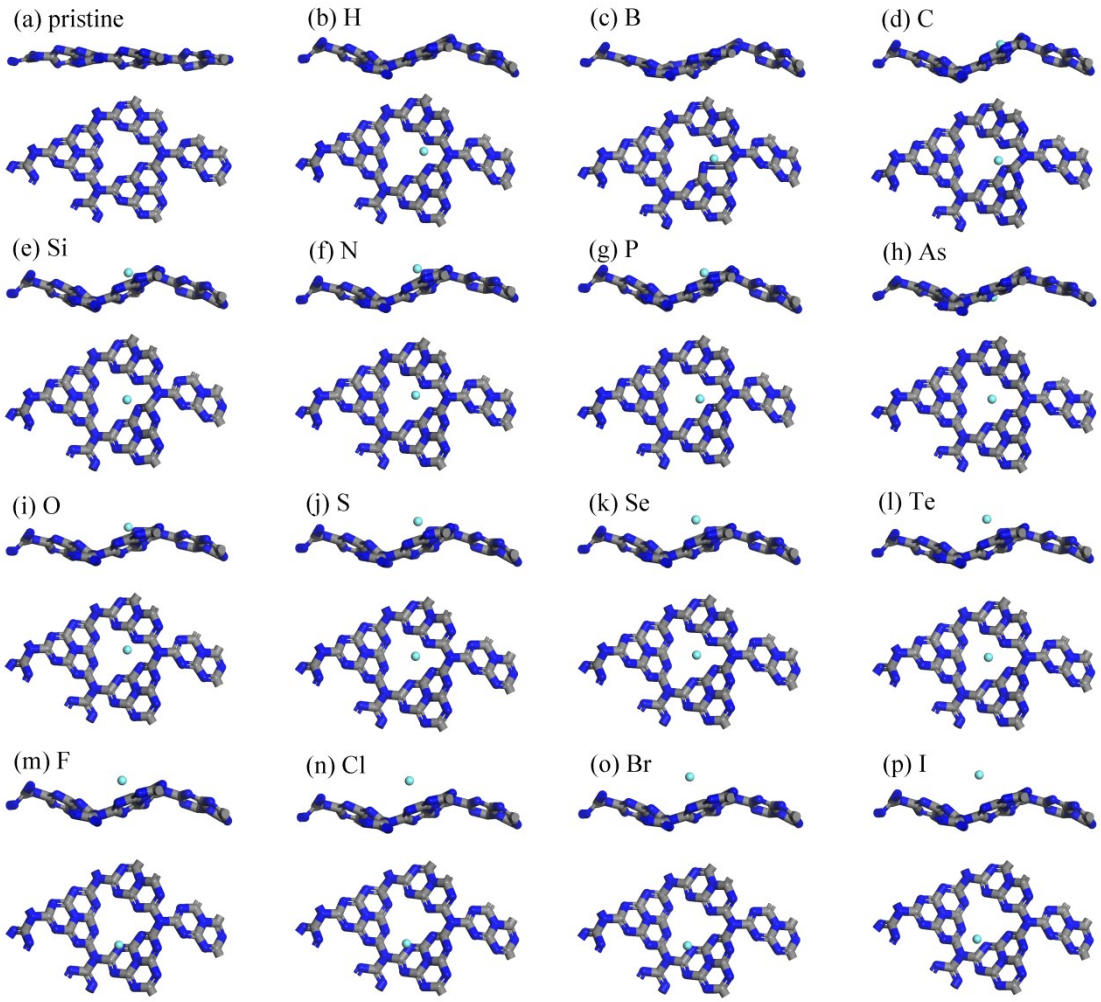

Figure S2. (Color online) The top and side views of (a) 2×2 pristine g–C_3N_4 monolayer and (b-p) the g–C_3N_4 monolayer after absorbing nonmetal atoms, where gray, blue and wathet spheres are the C, N and nonmetal atoms.

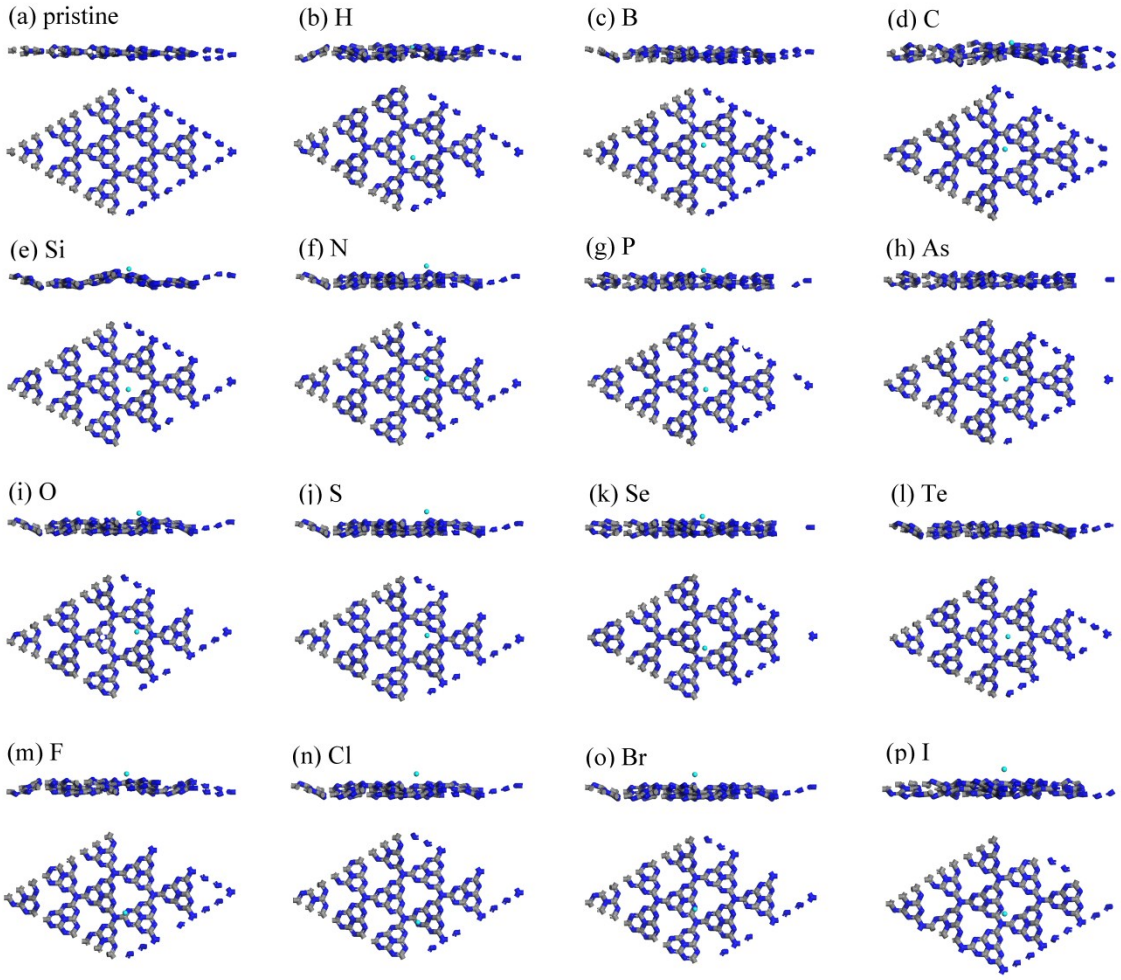

Figure S3. (Color online) The top and side views of (a) 3×3 pristine g–C_3N_4 monolayer and (b-p) the g–C_3N_4 monolayer after absorbing nonmetal atoms, where gray, blue and wathet spheres are the C, N and nonmetal atoms.

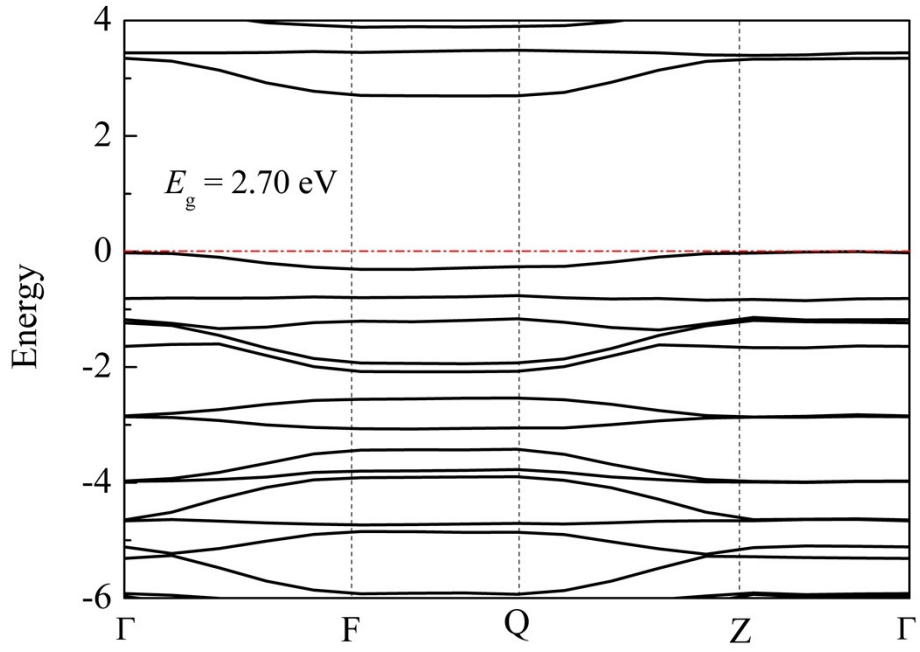

Figure S4. The band structure of pristine g–C_3N_4 monolayer with hybrid functional.

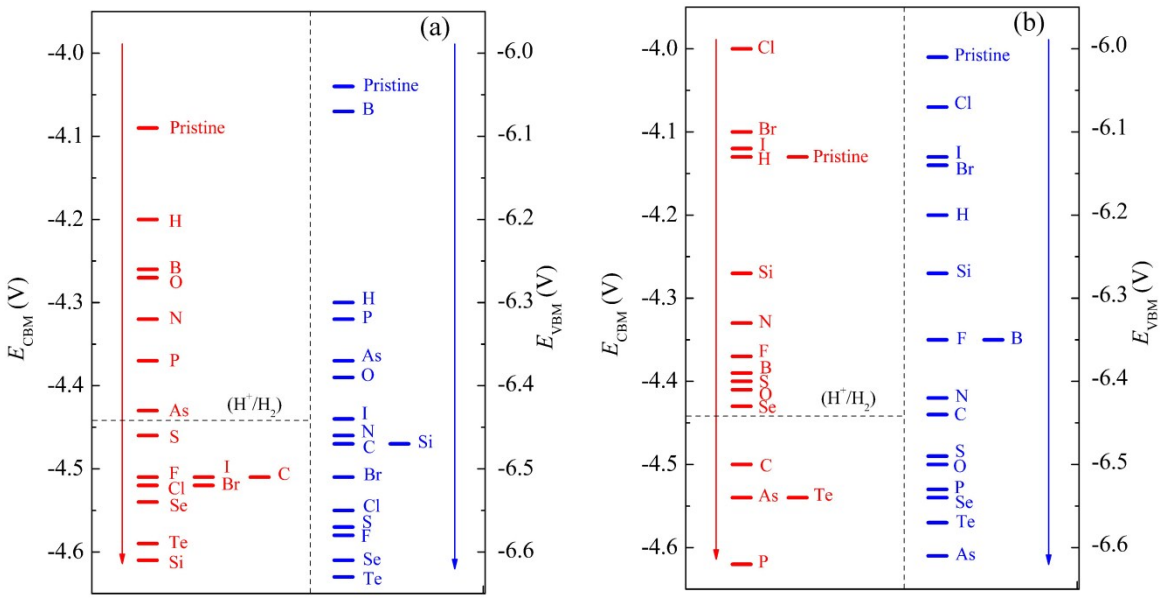

Figure S5. (Color online) The E_{CBM} and E_{VBM}, versus vacuum level of g–C_3N_4 monolayer before and after absorbing nonmetal atom for (a) 2×2 and (b) 3×3 specimens.

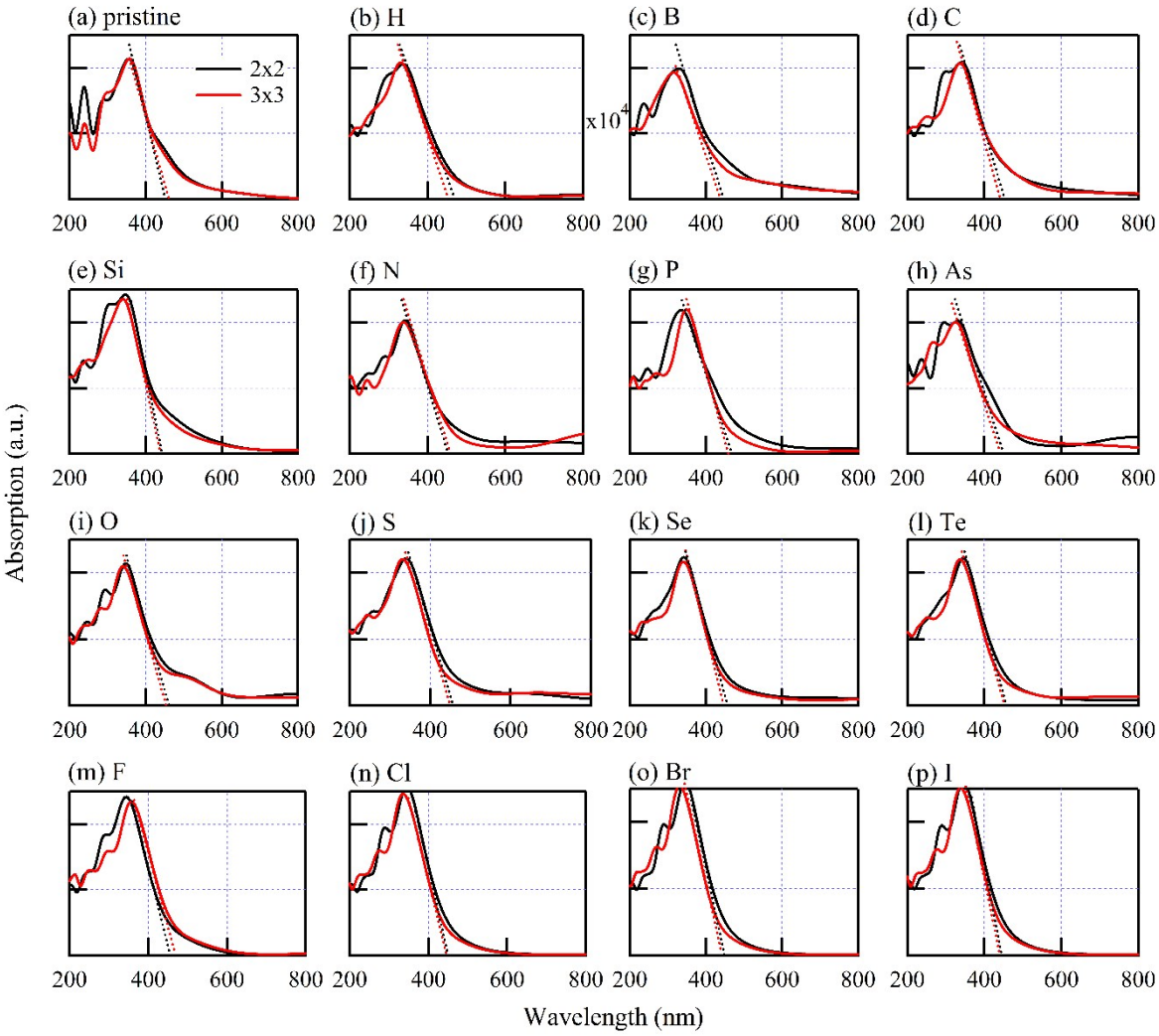

Figure S6. (Color online) The optical absorption curves of (a) pristine g–C_3N_4 monolayer and (b-p) g–C_3N_4 monolayer after absorbing nonmetal atoms for both 2×2 and 3×3 supercell specimens.