Supplementary Materials

The doping effects on antibonding states and carriers of two-dimensional PC_6

*Mi Zhong [a], Wei Zeng [b], Han Qin [c], Sheng-Hai Zhu [a], Xing-Han Li [a], Fu-Sheng Liu [a], Bin Tang [d], Qi-Jun Liu [a, *]*

[a] School of Physical Science and Technology, Southwest Jiaotong University, Chengdu 610031, People's Republic of China

[b] Teaching and Research Group of Chemistry, College of Medical Technology, Chengdu University of Traditional Chinese Medicine, Chengdu 610075, People's Republic of China

[c] School of Science, Xihua University, Chengdu 610039, People's Republic of China

[d] State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, People's Republic of China

Correspondence about the paper at the following address and e-mail address:

School of Physical Science and Technology, Southwest Jiaotong University, Chengdu, Sichuan 610031, People's Republic of China

Qi-Jun Liu, E-mail: qijunliu@home.swjtu.edu.cn

[*] Corresponding author. E-mail: qijunliu@home.swjtu.edu.cn

Contents:

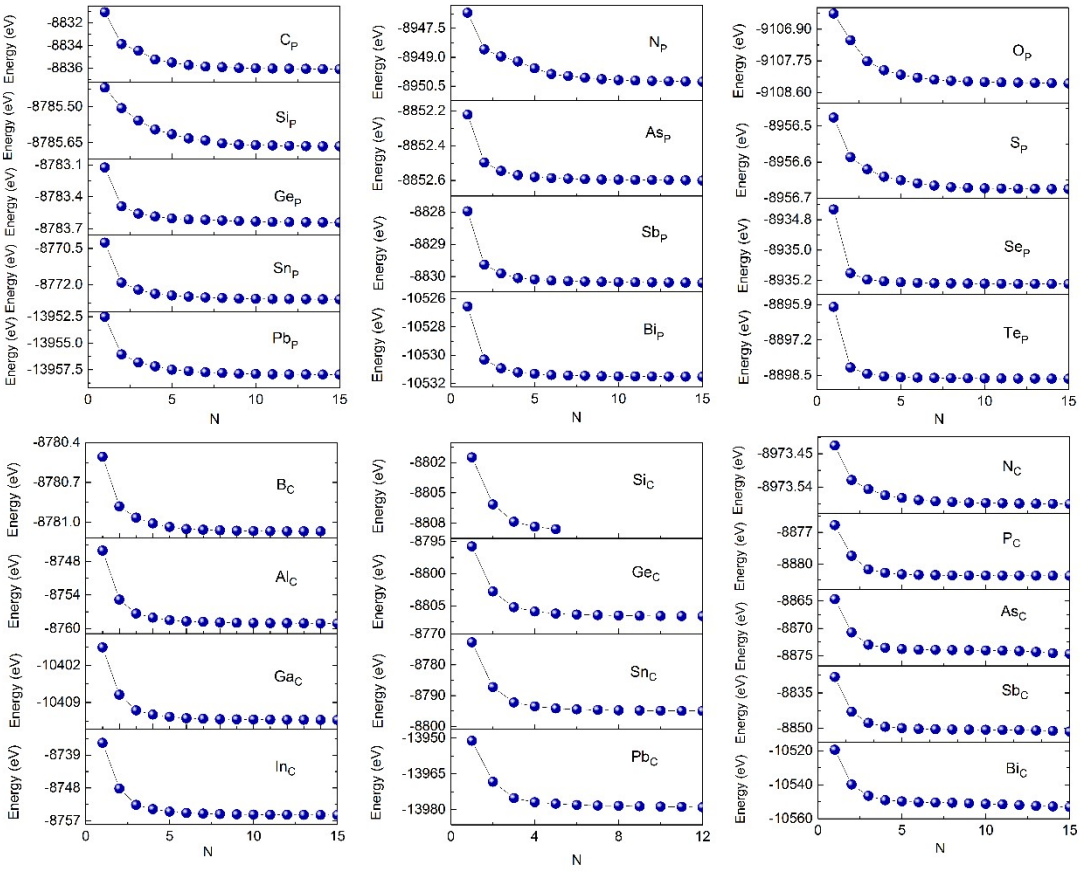

Figure S1. Calculated total energies as a function of N for the doped PC_6, N is optimization step.

Table S1 The optimized lattice constants, bond length, and bond angle of doped PC6 along with the pure system.

	a, b (Å)	d (Å)	θ (°)		a, b (Å)	d_1 (Å)	d_2 (Å)	θ_1 (°)	θ_2 (°)
pure	13.395, 13.395	1.804	98.173	pure	13.395, 13.395	1.360	1.804	116.697	125.000
IV group				III group					
C_P	13.373, 13.373	1.438	119.845	B_C	13.458, 13.419	1.488	1.860	117.427	126.122
Si_P	13.448, 13.448	1.733	108.339	Al_C	13.511, 13.400	1.848	2.212	113.997	112.399
Ge_P	13.407, 13.410	1.947	93.706	Ga_C	13.563, 13.444	1.858	2.195	120.643	115.677
Sn_P	13.398, 13.398	2.097	86.707	In_C	13.477,13.375	1.990	2.419	97.914	105.760
V group				IV group					
N_P	13.330, 13.330	1.427	119.802	Si_C	13.529, 13.427	1.716	2.129	119.125	117.947
As_P	13.397, 13.397	1.922	93.096	Ge_C	13.479, 13.427	1.933	2.353	101.223	92.487
Sb_P	13.401, 13.401	2.059	88.118	Sn_C	13.436, 13.381	2.104	2.675	71.609	87.703
VI group				V group					
O_P	13.360, 13.358	1.532	116.691	N_C	13.370, 13.389	1.378	1.781	116.527	125.201
S_P	13.414, 13.414	1.790	101.012	P_C	13.480, 13.417	1.750	2.192	108.072	104.149
Se_P	13.422, 13.422	1.915	96.127	As_C	13.488, 13.418	1.877	2.285	104.167	97.430
Te_P	13.424, 13.424	2.071	90.213	Sb_C	13.490, 13.412	2.021	2.433	99.379	90.945

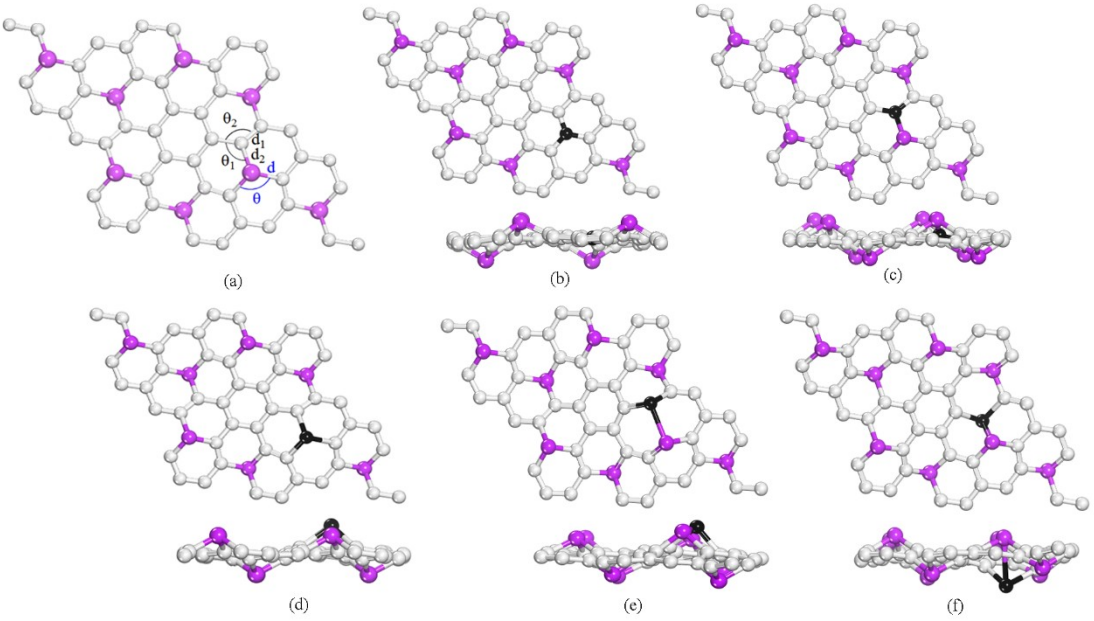

Figure S2. The top and side views of the doped PC_6, dopants in black. (a) the bond length and bond angel corresponding to the ones in Table 1. (b) P-site substituted systems with carbon-coplanar dopants (C, N, and O atoms). (c) C-site substituted systems with carbon-coplanar dopants (Si, N, B, Al and Ga). (d) P-site substituted systems with dopants above the carbon-plane dopants (Si, Ge, Sn, As, Sb, S, Se, Te). (e) C-site substituted systems with dopants above the carbon-plane (Ge, P, As and Sb atoms). (f) C-site substituted systems with dopants below the carbon plane (In and Sn atom).

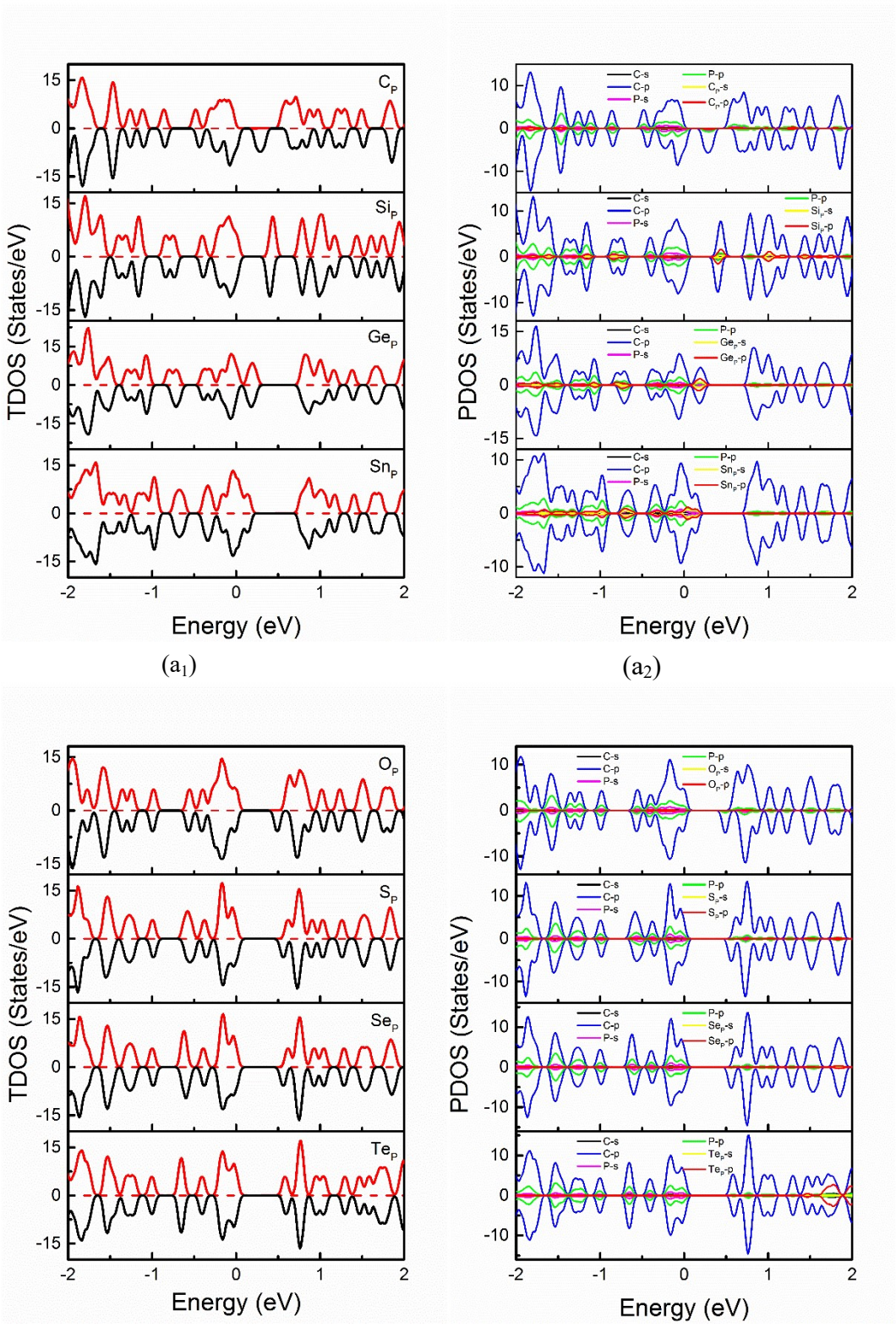

Figure S3. (a_1) and (b_1) The total density of states (TDOS) for the X-doped PC_6. (a_2) and (b_2) Partial density of states (PDOS) for the X-doped PC_6. X dopants from group IV and VI. In TDOS, the red line is for spin-up states and the black line is for spin-down states.

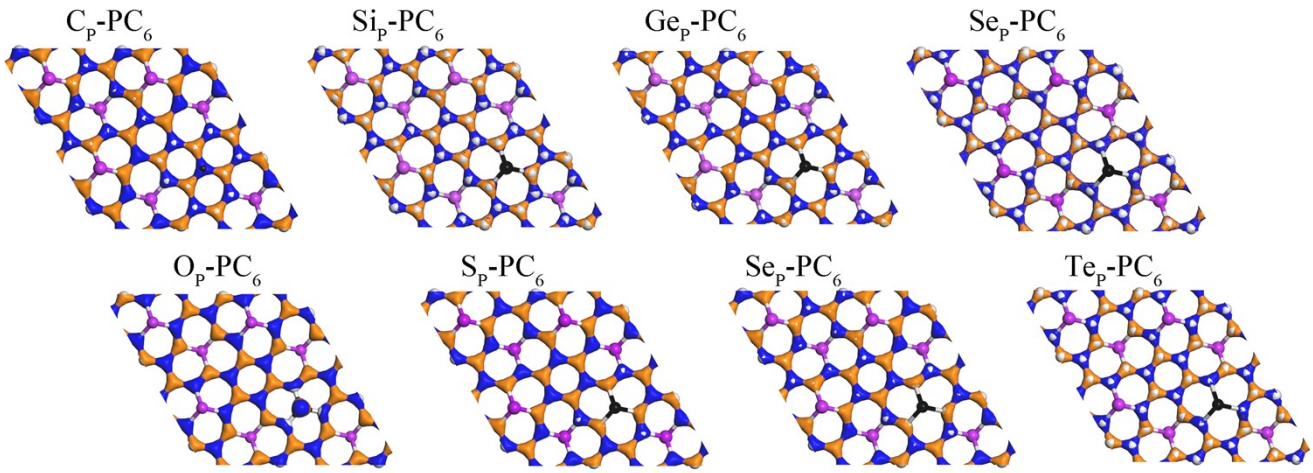

Figure S4. Spatial spin density distributions of the group IV and VI substitutional doped PC_6 (Yellow/blue color represents the spin-up/down density distributions).

Table S2. The actually Fermi energy ($E_{F'}$) and normalized position of Fermi level.

Systems	$E_{F'}$	E_F
Pure	-2.55	0.00
O_P	-2.19	0.36
S_P	-2.20	0.36
Se_P	-2.17	0.39
Te_P	-2.12	0.43
N_C	-2.30	0.25
P_C	-2.35	0.20
As_C	-2.29	0.26
Sb_C	-2.32	0.23