Supplementary Information

The Role of Local Orbital Hybridization in Band Gap Opening and Magnetism Induced by Single-Atom Doping in Graphene

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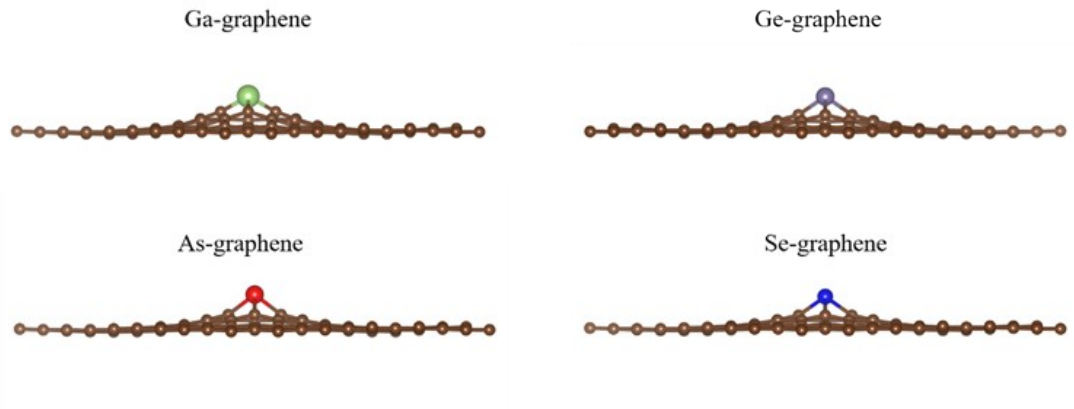

Fig. S1 Side view of the optimized configurations for Ga-, Ge-, As-, and Se-doped graphene with fully cell relaxation.

Table S1 Differences in total energy (per atom), hybrid bond length, and lattice constant between fixed and fully relaxed cell geometry optimization.

	Total energy (meV)	Hybrid bond length (Å)	Lattice constant (Å)
Ga-graphene	-4.86	0	0.01
Ge-graphene	-5	0	0.01
As-graphene	-4.58	0	0
Se-graphene	-5	0	0.02

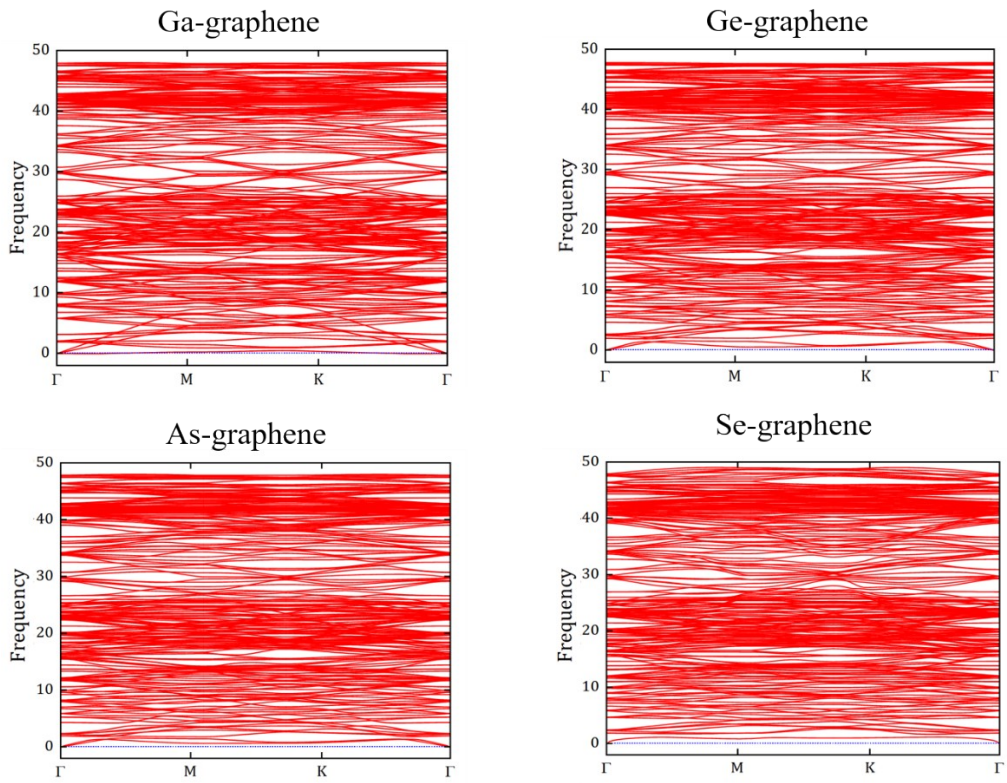

Fig. S2 Phonon spectra of Ga-, Ge-, As- and Se-doped graphene systems.

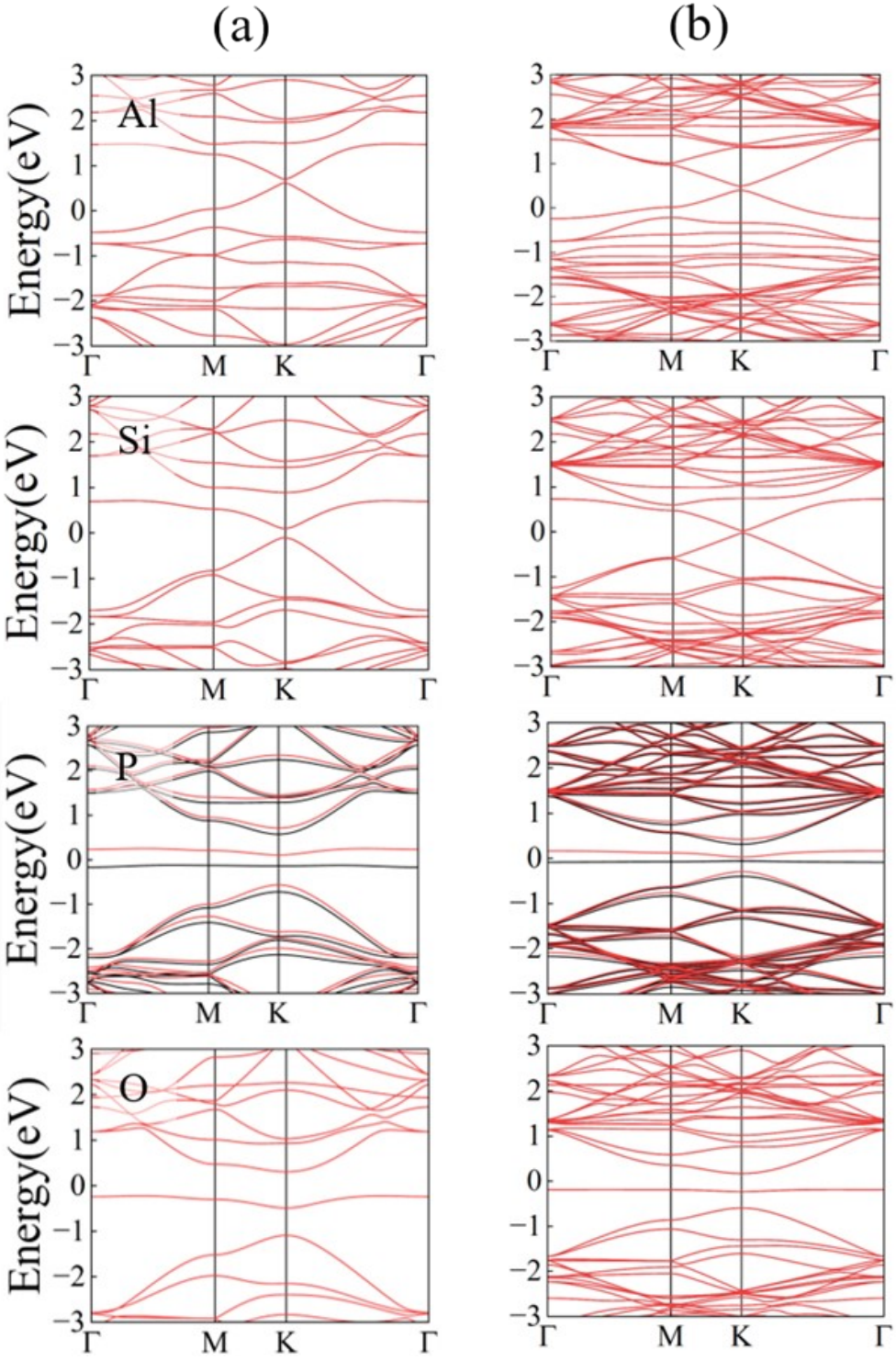

Fig. S3 Spin-polarized band structures at (a) 3.1% and (b) 1.0% doping concentrations for Al- Si-, P-, and O-doped graphene.

Table S2 Band gap values at different doping concentrations in Al- Si-, P-, and O-

doped graphene.

	Band gap (eV)		
	4 × 4 (3.1%)	6 × 6 (1.4%)	7 × 7 (1.0%)
Al-graphene	0.030	0.004	0.013
Si- graphene	0.191	0.014	0.039
P- graphene	0.693	0.008	0.352
O- graphene	0.525	0.013	0.354

Table S3 Band gap values obtained by PBE and HSE06 hybrid functional calculations.

	Band gap (eV)	
	PBE	HSE06
Al-graphene	0.004	0.014
Si- graphene	0.014	0.067
P- graphene	0.008	0.042
O- graphene	0.013	0.022

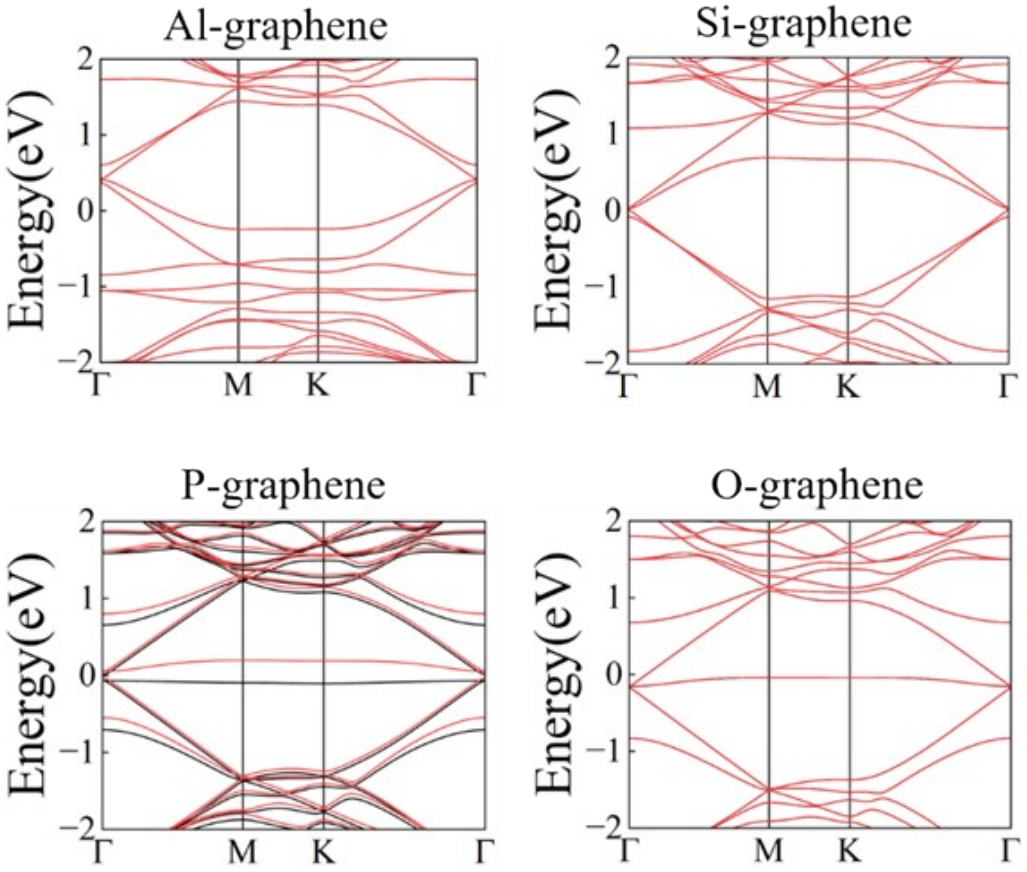

Fig. S4 Band structure diagram obtained by HSE06 hybrid functional calculations.