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Doping Effect on Catalytic Activity of Graphene for Oxygen Evolution Reaction in Lithium−Air Battery: A First-Principles Study

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Table S1. The formation energies of all doped graphenes; the formation energy is calculated by $\Delta E_F = E - N_C U_C - N_X U_X - N_H U_H$, where N_C and N_X are the total number of C and X atoms in the cell calculated; U_C and U_X are the chemical potential of C and X. We take CH_4 as the reference of C potential, and other potential references of X are listed.

Systems	**Graphene**	**B-doped**	**N-doped**	**Si-doped**	**Al-doped**	**P-doped**	**B,P-codoped**
Formation energy (eV)	0.885	0.893	0.901	0.936	0.968	0.917	0.907
References	CH_4	CH_4, BH_3	CH_4, NH_3	CH_4,Si (silicon)	CH_4, Al(metal)	CH_4, P(white P4)	CH_4, BH_3, P(white P4)

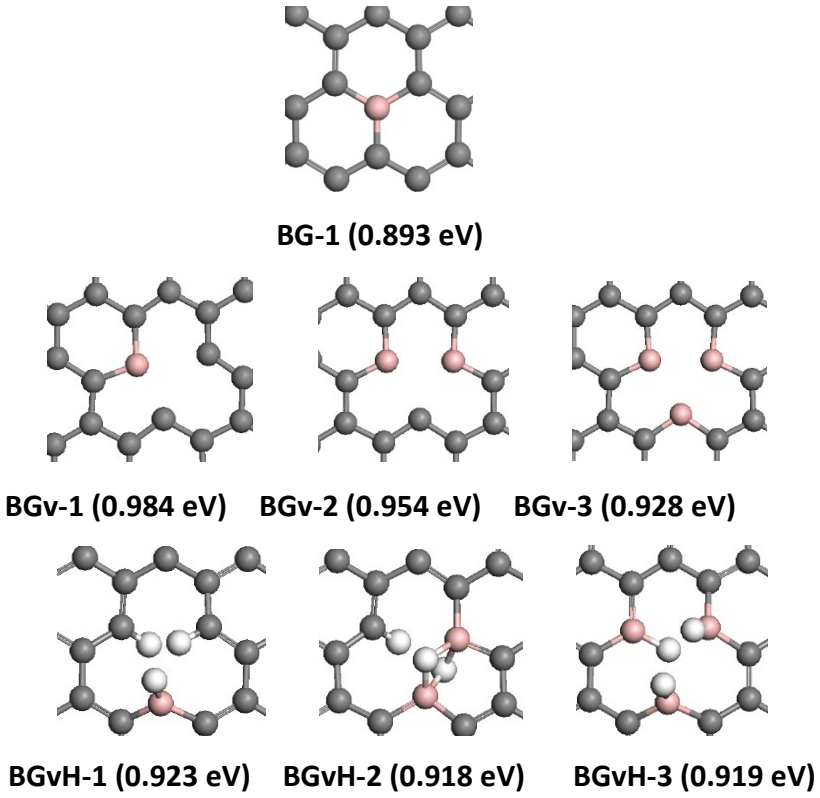


Figure S1. All relaxed structures for B-doped graphene and their corresponding formation energies in parentheses. The formation energy is calculated by the equation in Table S1.

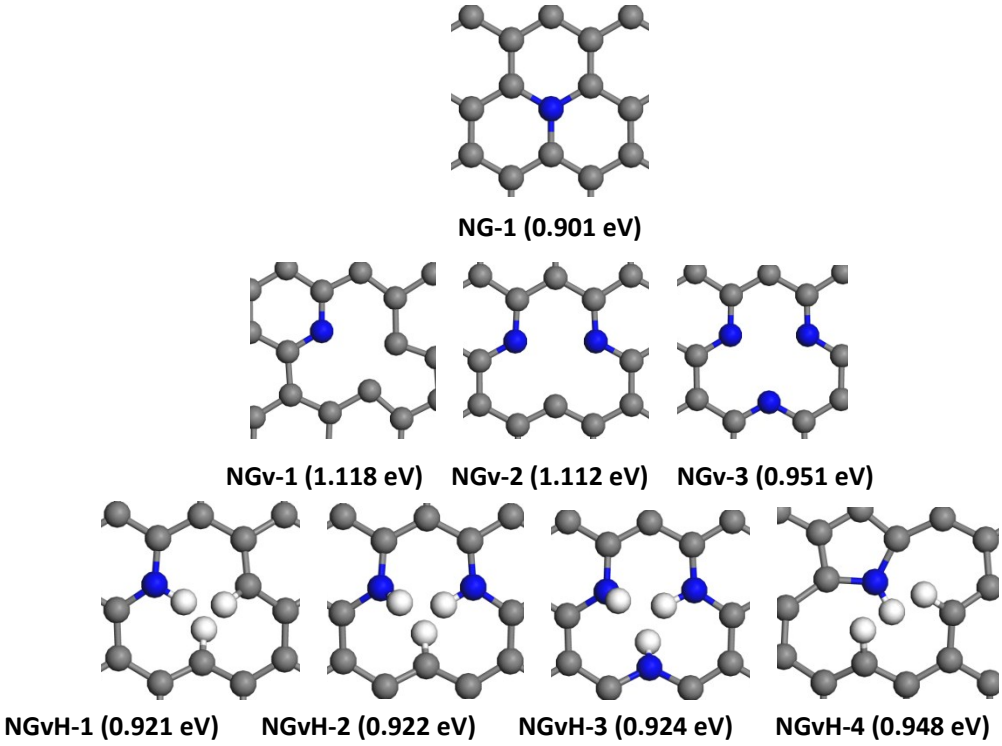


Figure S2. All relaxed structures for N-doped graphene and their corresponding formation energies in parentheses. The formation energy is calculated by the equation in Table S1.

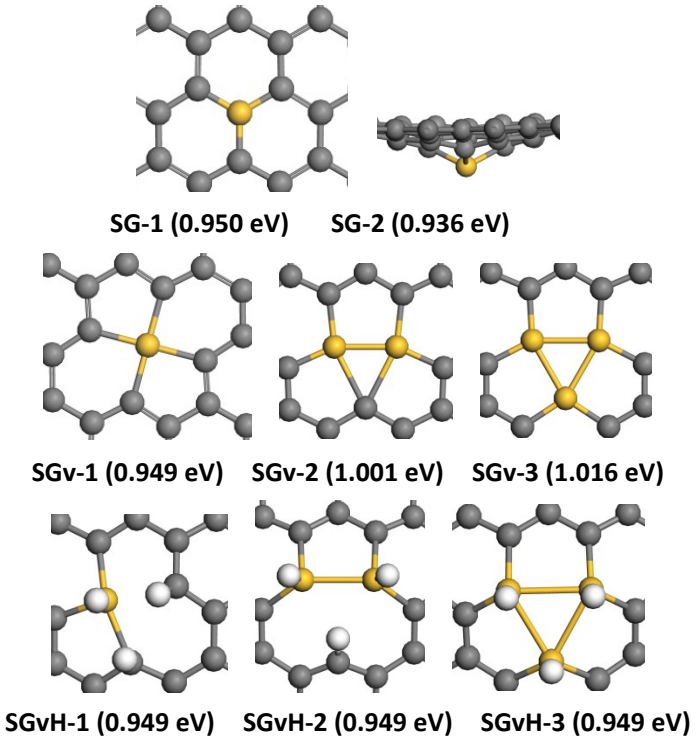


Figure S3. All relaxed structures for Si-doped graphene and their corresponding formation energies in parentheses. The formation energy is calculated by the equation in Table S1. The SG-1 structure is the planar Si-doped structure, The SG-2 is the rippled sp^3 structure, and the SGv-1 is the sp^2d structure mentioned in the main text. SGvH-1, 2 and 3 are structures with carbon vacancy and H passivation atoms (white balls).

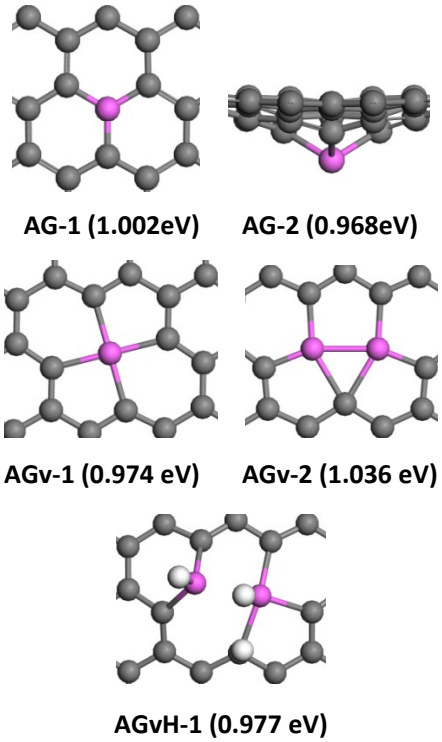


Figure S4. All relaxed structures for Al-doped graphene and their corresponding formation energies in parentheses. The formation energy is calculated by the equation in Table S1.

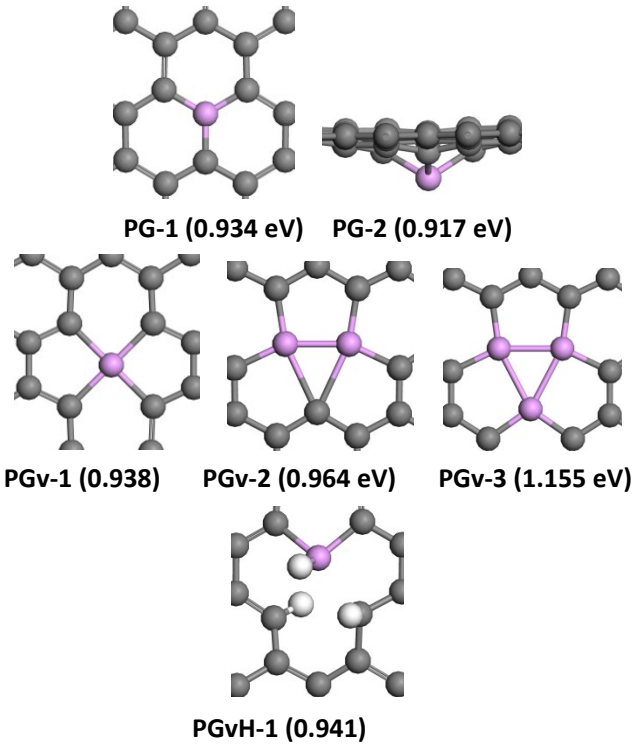
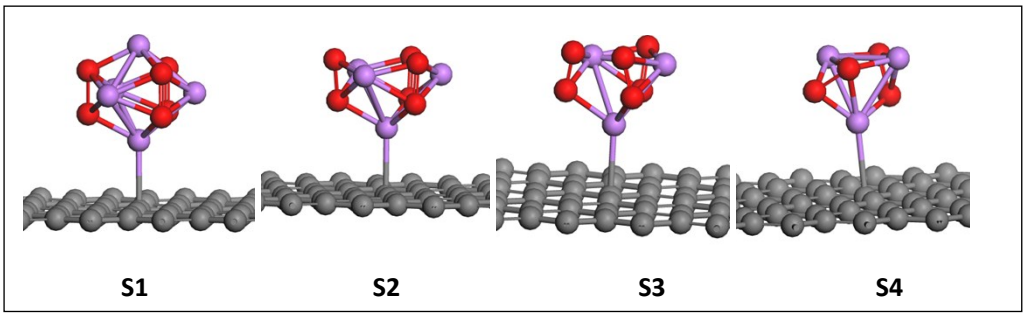
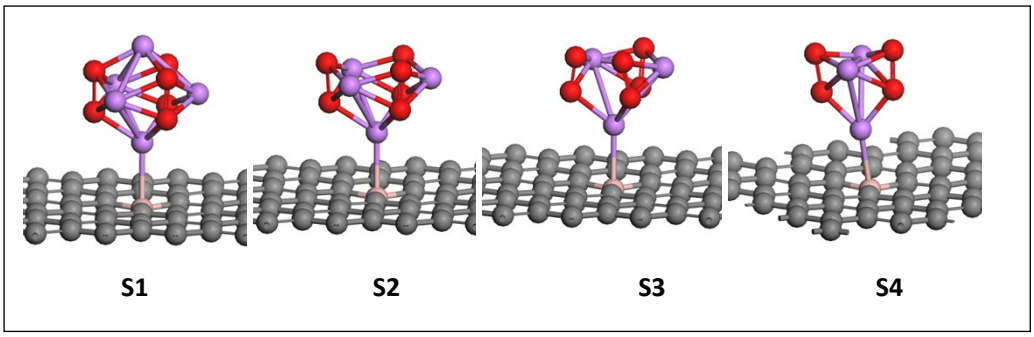


Figure S5. All relaxed structures for P-doped graphene we calculated and their formation energies in parentheses. The formation energy is calculated by the equation in Table S1.

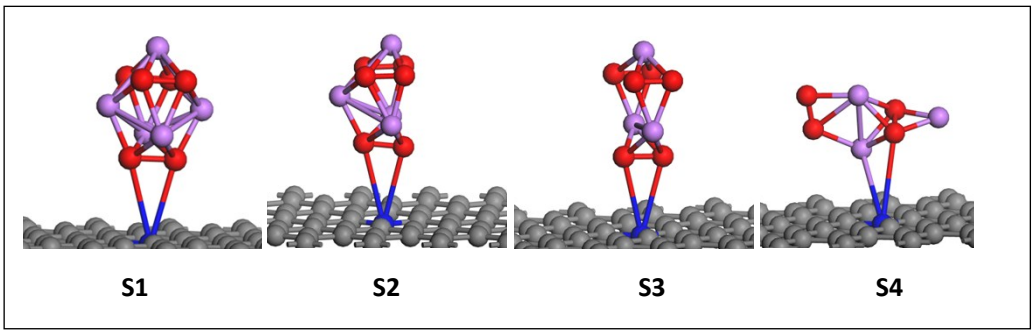
Pathway on Graphene



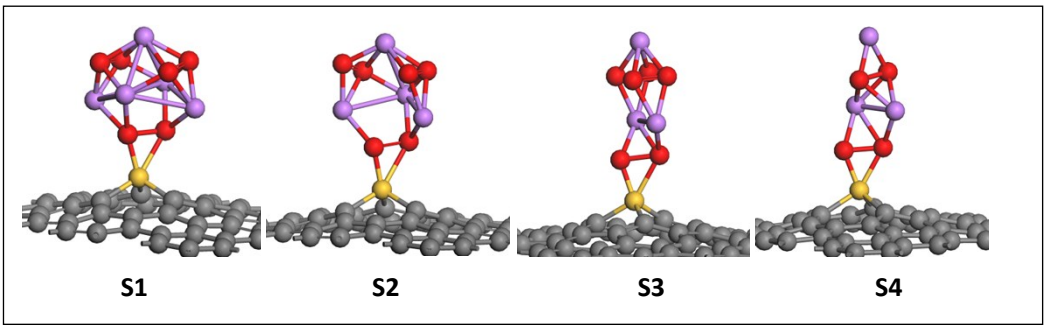
Pathway on B-doped Graphene



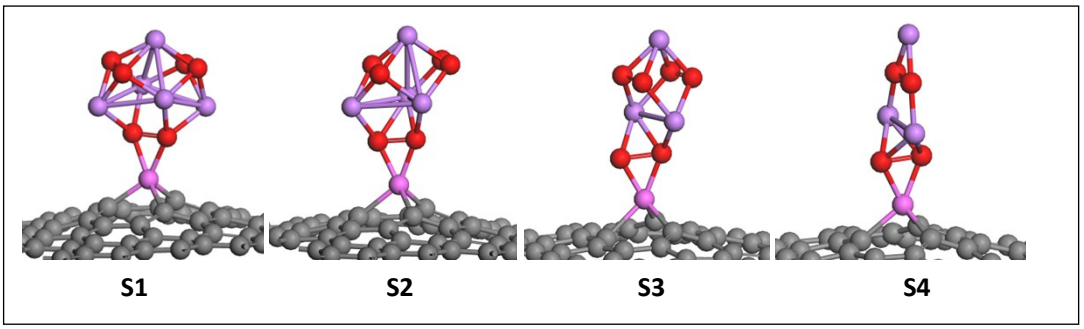
Pathway on N-doped Graphene



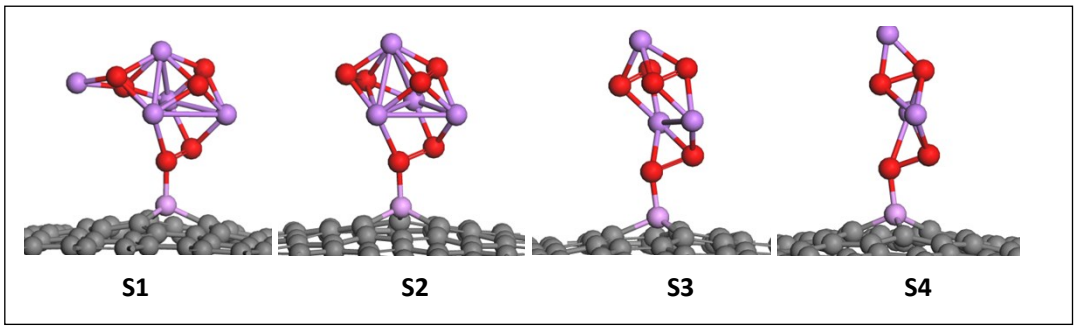
Pathway on Si-doped Graphene



Pathway on Al-doped Graphene



Pathway on P-doped Graphene



Pathway on B-P co-doped Graphene

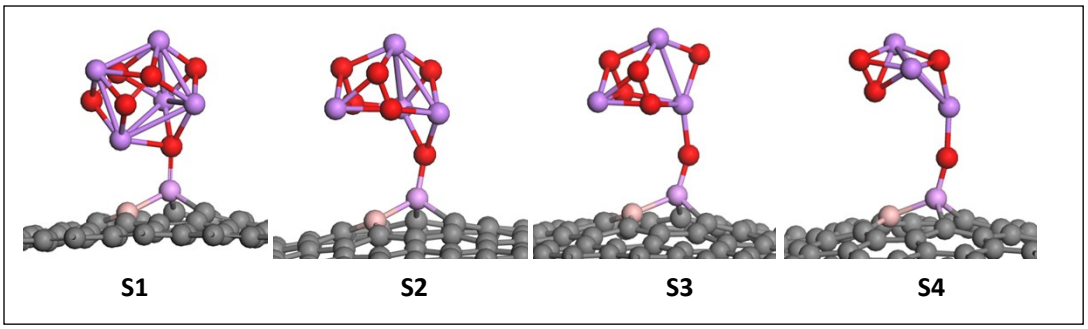
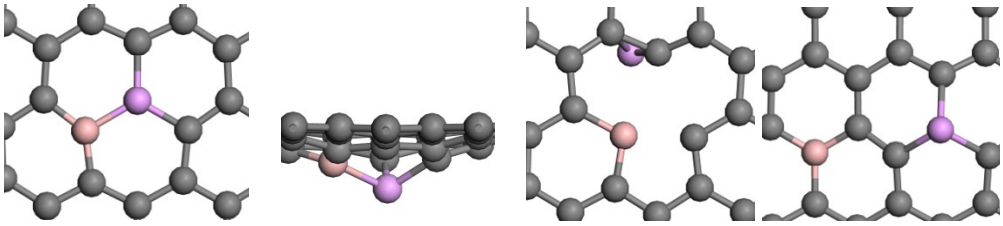


Figure S6. The calculated OER pathways on all doped graphene materials



BPG-1 (0.926 eV) **BPG-2 (0.907 eV)** **BPG-3 (0.982 eV)** **BPG-4 (0.909 eV)**

Figure S7. All relaxed structures for B,P-codoped graphene we calculated and their formation energies in parentheses. The formation energy is calculated by the equation in Table S1. BPG-1 structure is the planar adjacent structure; the BPG-2 is the rippled structure; the initial structure of BPG-3 is the para-isomer structure for B,P-codoped graphene but it is not stable; BPG-4 is the third adjacent structure.