Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The mechanisms of the direct synthesis of hydrogen peroxide on silicon and phosphorus dual doped graphene: A DFT-D study

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We firstly considered that the Si and P replace two C atoms and all substrates (included type-I, type-II and type-III) are relaxed, as shown in Fig. S1. The most stable structures of type-I, type-II and type-III are in the leftmost column.

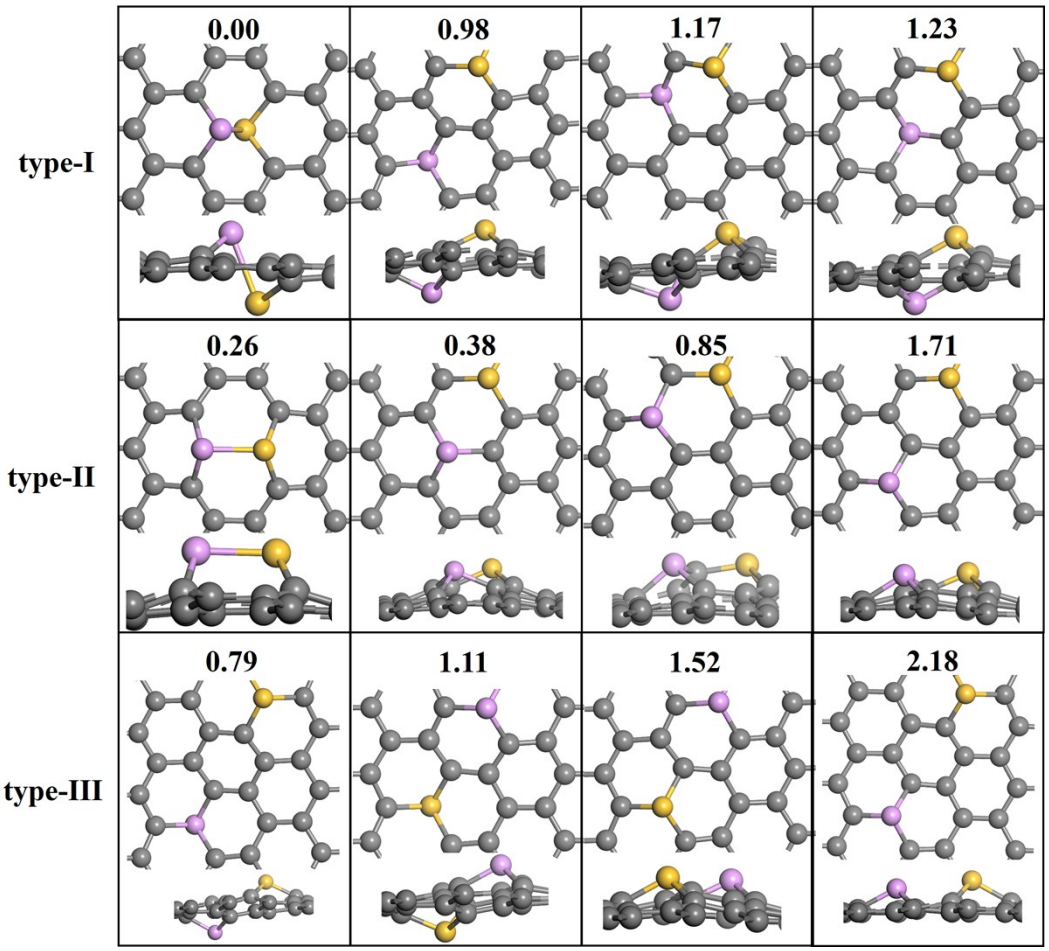

Fig. S1 Atomic structures of relaxed structures for the various ORR chemical species adsorbed on Si-G-P. Gray, yellow and pink spheres represent C, Si and P atoms, respectively. The relative energy (eV) is marked in figures with the first substrate's energy for the zero potential energy.

The first substrate is selected for the adsorption of O_2, as shown in Fig. S2. We find that the formation PO_2 species taken out the surface, indicating that Si is doped the defect graphene. A similar situation would still appear when the O_2 is prepositioned on the Si atom. The O_2 molecule would pull the Si atoms out of the surface.

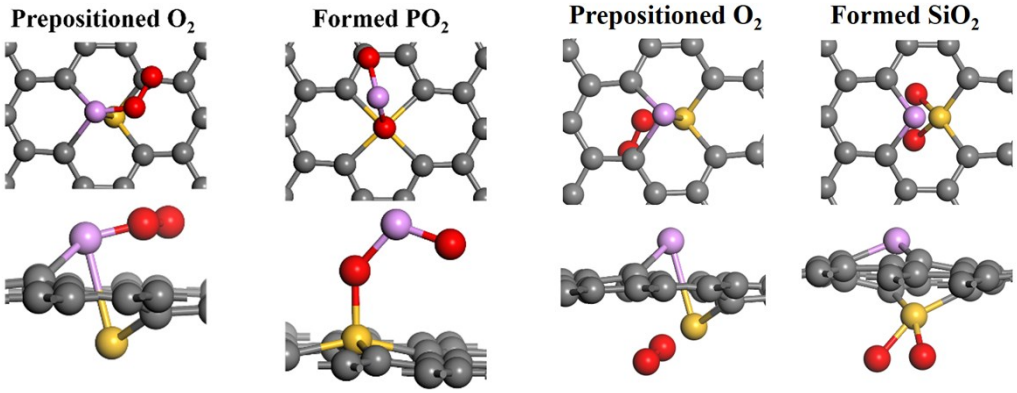

Fig. S2 The O_2 molecule adsorbed on the relaxed substrate. The prepositioned O_2 is on left, while the relaxed configuration is on right. Gray, yellow, pink and red spheres represent C, Si, P and O atoms, respectively.

All designed possibilities are calculated for selecting the most stable selected substrates, as shown in Fig. S3. We find that the most stable substrate is formed the doped center of the Si dopant and the phosphorus dopant is neighbor with the atomic Si.

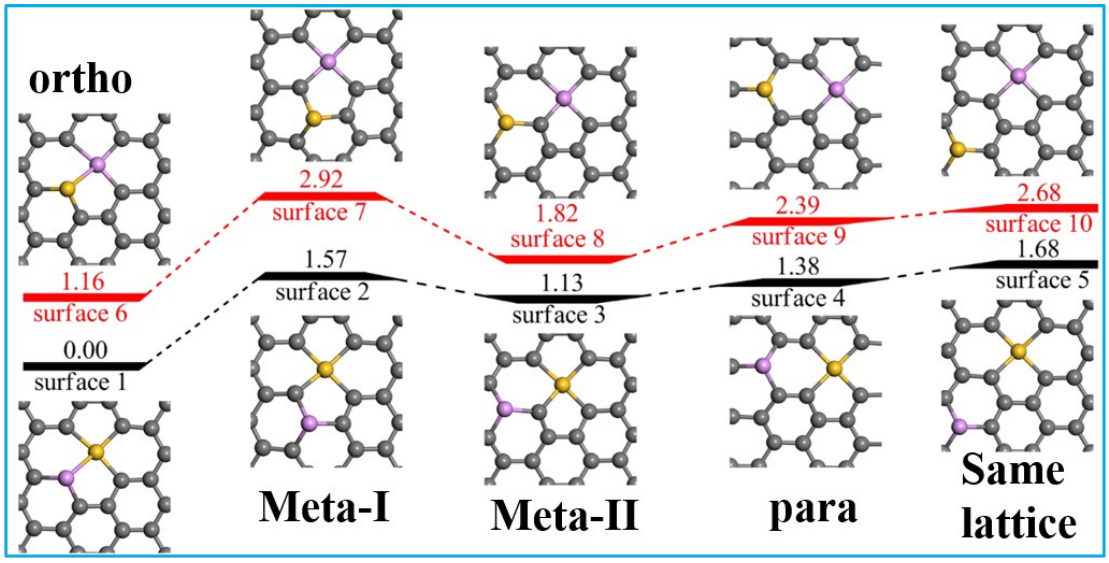

Fig. S3 The dopant center of silicon and phosphorus is doped into graphene with the different substrate named ortho, meta-I, meta-II, para and same lattice (marked as "surface 1~10"). Gray, yellow and pink spheres represent C, Si and P atoms, respectively. The relative energy (eV) is marked in figures with the most stable substrate's energy for the zero potential energy.