Supporting Information for

Catalytic CO oxidation on B-doped and BN co-doped penta-graphene: A computational study

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Figure S1. Optimized configurations and calculated formation energies of different B-doped and BN co-doped penta-graphene: (a) for different B-doped PG penta-graphene and (b), (c), (d), (e), (f) for different BN co-doped penta-graphene.

Figure S2. Optimized adsorption configurations: (a) O$_2$, (b) CO, (c) atomic O, (d) CO$_2$ at C=C site of the B-doped PG, and (e) pre-adsorption of CO on adsorbed O$_2$, (f) co-adsorption of O$_2$ and CO, and (g) co-adsorption of two CO at B=C site of the B-doped PG.
Figure S3. Optimized adsorption configurations: (a) $O_2$, (b) CO, (c) atomic O, (d) $CO_2$ at C=C site of the BN co-doped PG, and (e) pre-adsorption of CO on adsorbed $O_2$ and (f) co-adsorption of $O_2$ and CO at B=N site of the BN co-doped PG.

Figure S4. Minimum energy paths calculation for $O_2$ reduction process on (a) the B=C site and (b) the C=C site of B-doped penta-graphene.

Figure S5. Minimum energy paths calculation for $O_2$ reduction process on (a) the B=N site and (b) the C=C site of BN co-doped penta-graphene.
Figure S6. Minimum energy paths calculation for CO adsorption process on (a) the B=C site of B-doped penta-graphene and (b) the B=N site of BN co-doped penta-graphene.

Figure S7. The optimized configurations including predicted adsorption energies for $O_2$ adsorption the various doping concentration of PG (a) $B_2C_{22}$, (b) $B_3C_{21}$, (c) $B_4C_{20}$, (a') $B_2N_2C_{20}$, (b') $B_3N_3C_{18}$, and (c') $B_4N_4C_{16}$. 