

Supplementary Materials: Theoretical Study on the Quantum Capacitance Origin of Graphene Cathodes in Lithium Ion Capacitors

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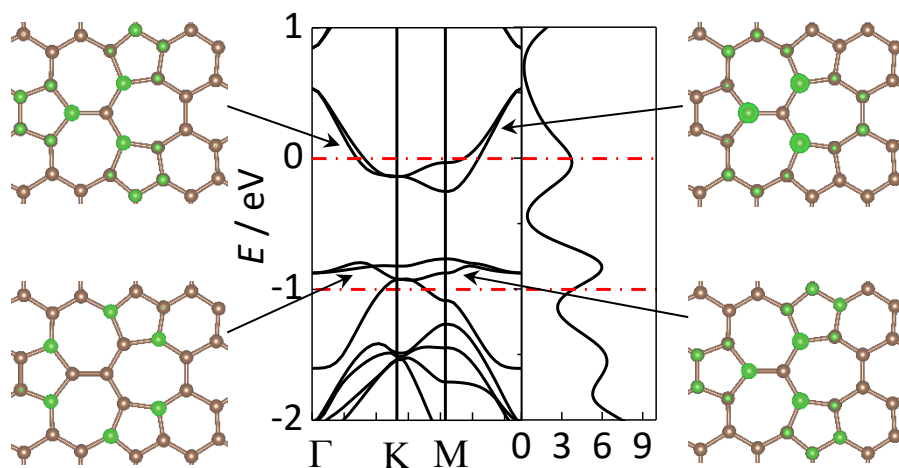


Figure S1. Band structure, DOS and band-decomposed charge density iso-surfaces ($0.003 e/\text{Bohr}^3$) of D2_II defected graphene.

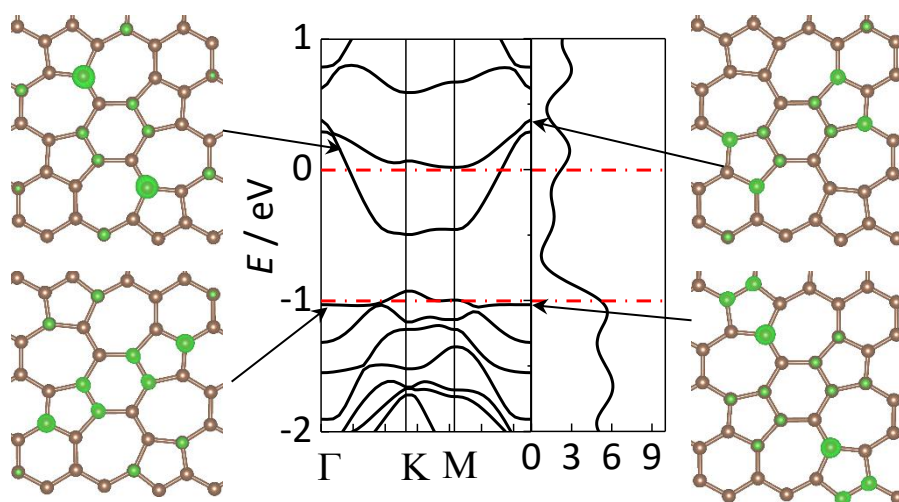


Figure S2. Band structure, DOS and band-decomposed charge density iso-surfaces ($0.003 e/\text{Bohr}^3$) of D2_III defected graphene.

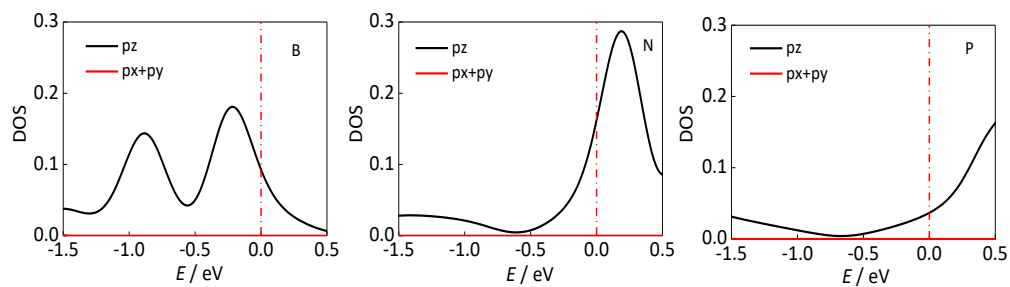


Figure S3. Split DOS of alien atoms in B, N and P doped graphene.

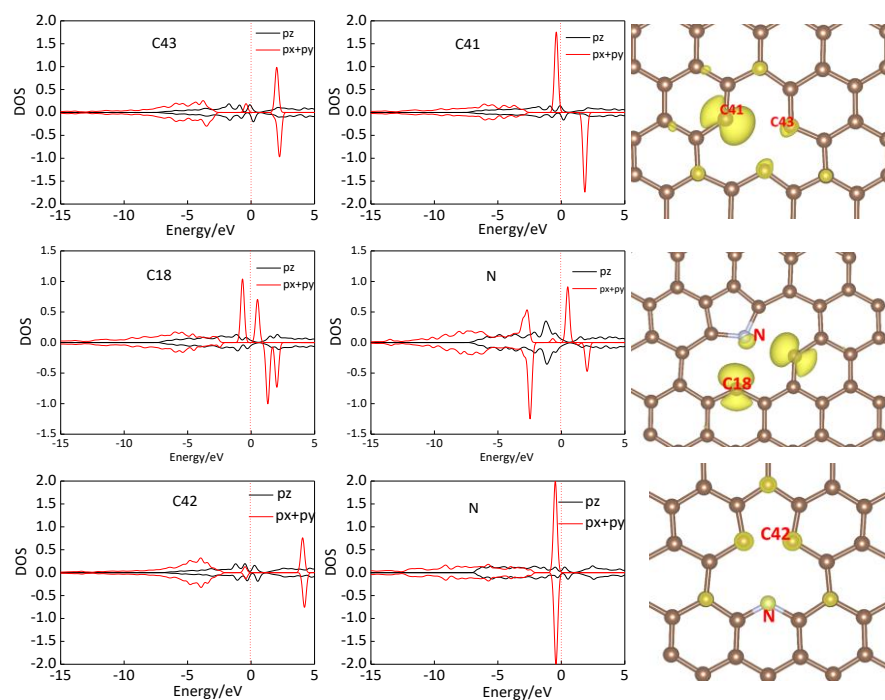


Figure S4. Split DOS and spin density of D1 defected graphene and graphene with pyrrolic and pyridinic N.

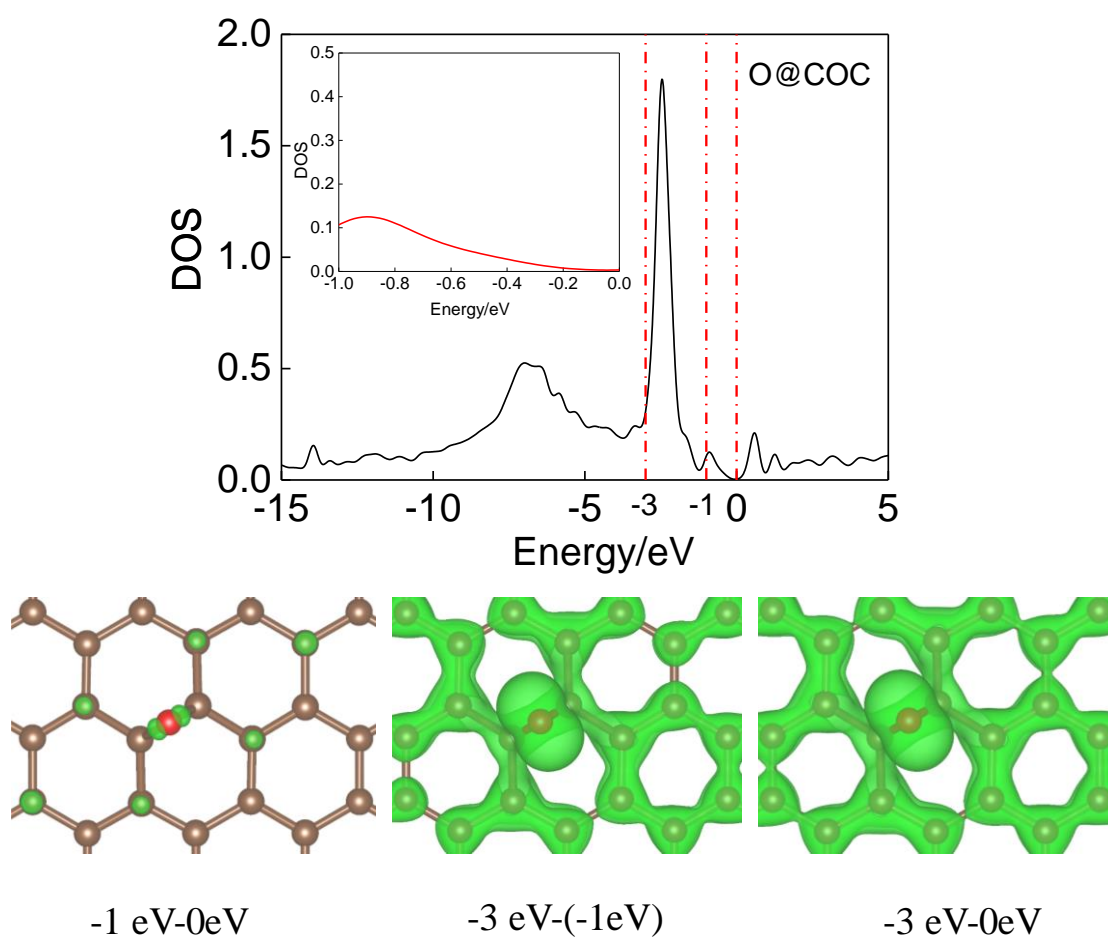


Figure S5. Split DOS of O in -COC- group and the band-decomposed charge density iso-surfaces (0.01 e/Bohr³) at different energy range.

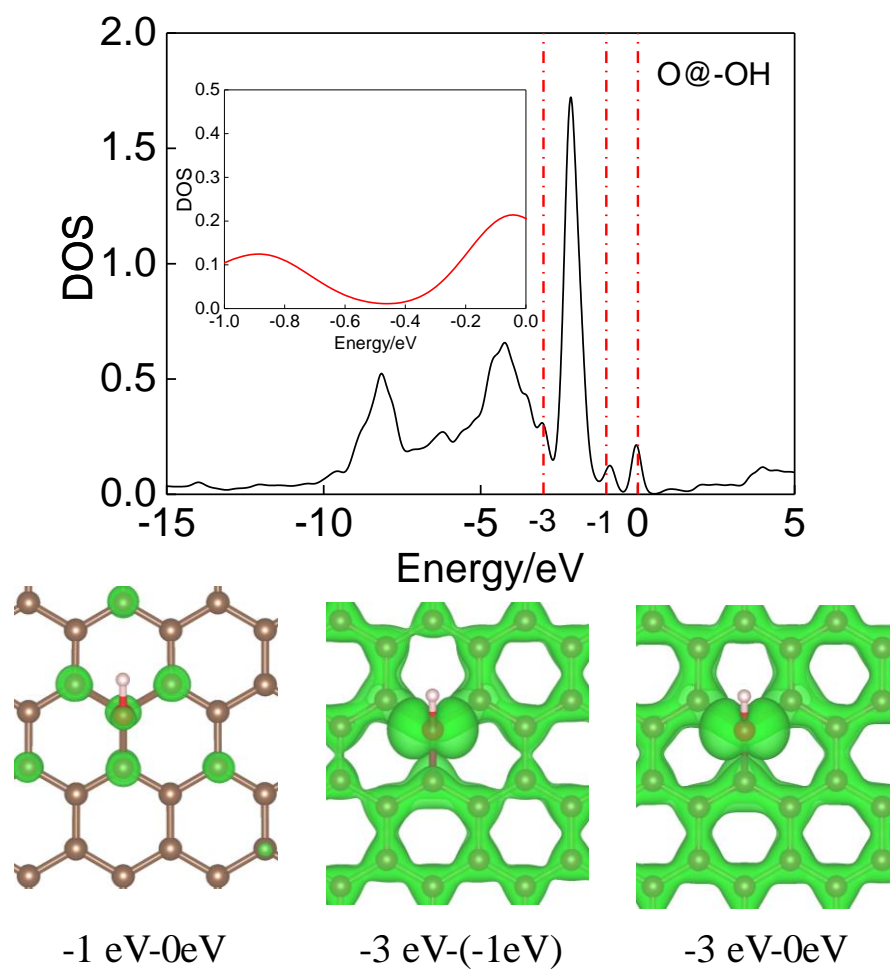


Figure S6. Split DOS of O in -OH group and the band-decomposed charge density iso-surces (0.01 e/Bohr³) at different energy range.