Electronic supplementary information

Rectangular and Hexagonal Doping of B, N, and O in Graphene: A DFT Study

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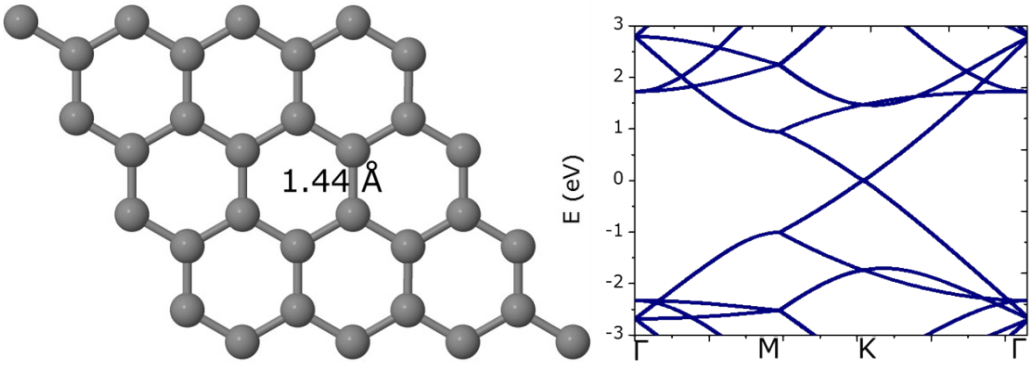

Figure S1: *Optimized geometry of graphene along with its corresponding band structure. The conduction and valence band touched at Dirac point. The Fermi energy is set to zero.*

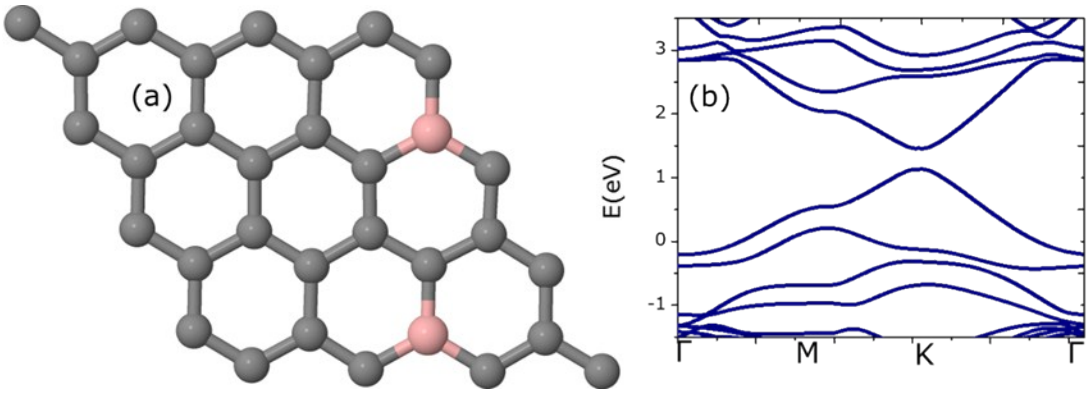

Figure S2: *Optimized geometry of graphene sheet doped with two B atoms at rectangular sites (a) along with the corresponding band structure graph (b)*

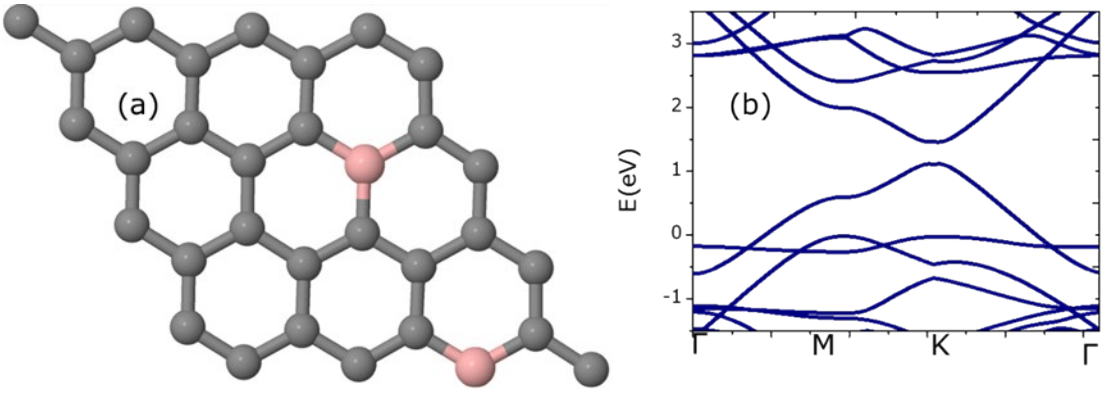

Figure S3: *Optimized geometry of graphene sheet doped with two B atoms at hexagonal sites (a) along with the corresponding band structure graph (b)*

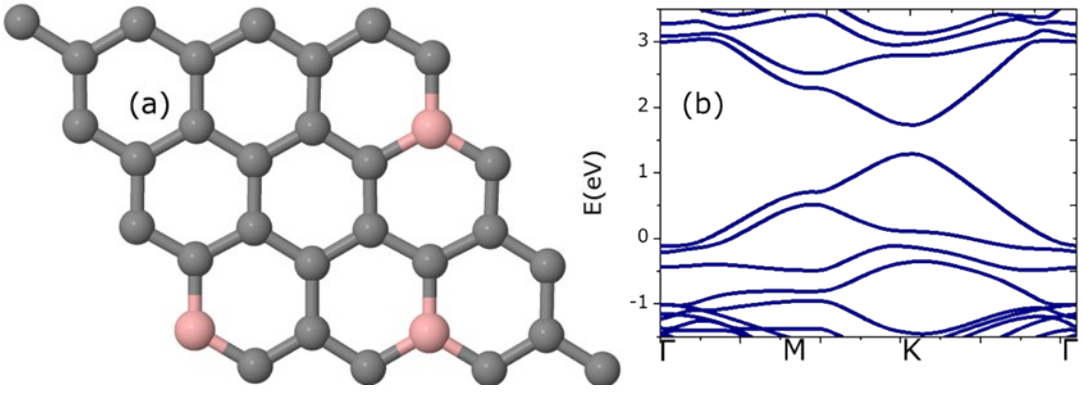

Figure S4: *Graphene sheet doped with three B at rectangular sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

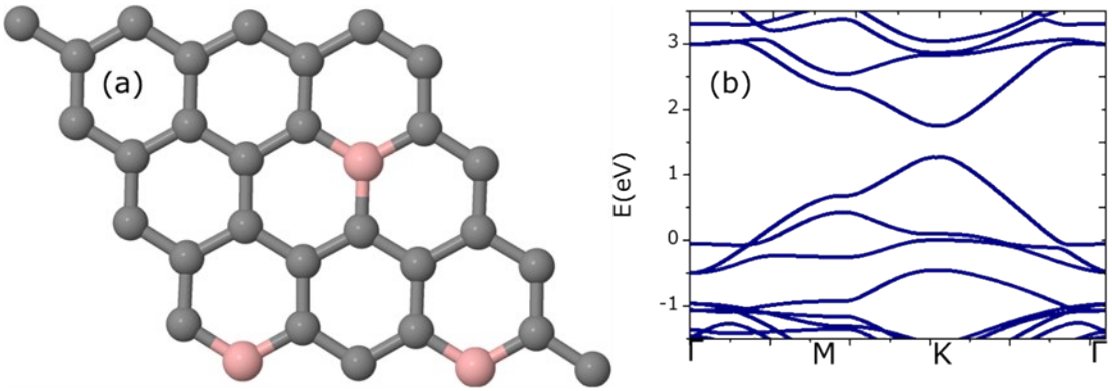

Figure S5: *Graphene sheet doped with three B at hexagonal sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

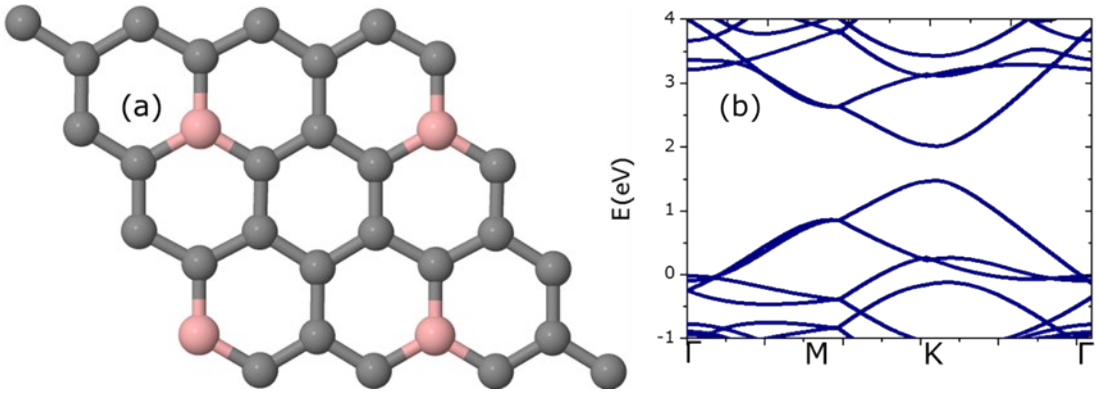

Figure S6: *Four B atoms doped in graphene sheet (rectangular configuration) is depicted in (a). The band structure graph is drawn in (b)*

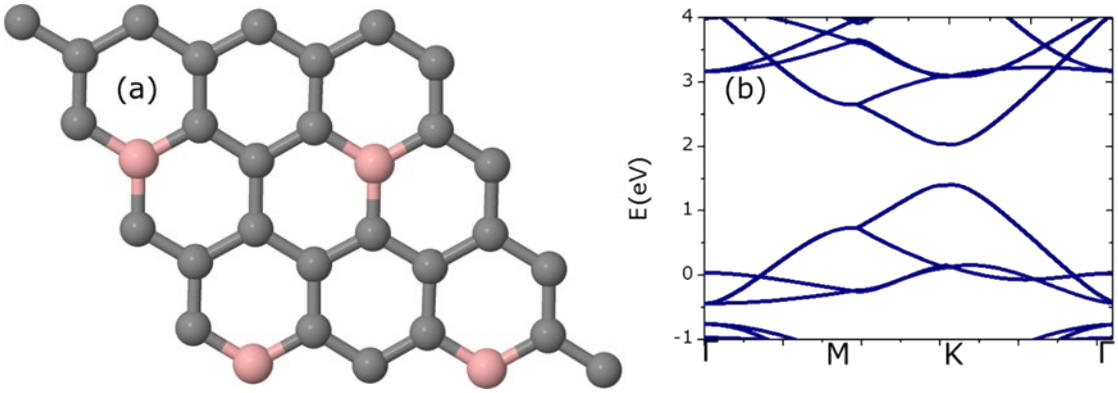

Figure S7: *Four B atoms doped in graphene sheet (hexagonal configuration) is depicted in (a). The band structure graph is drawn in (b)*

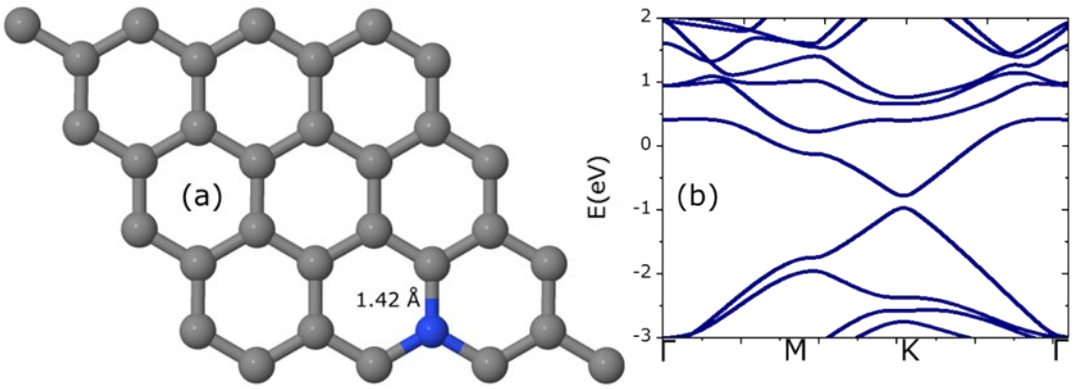

Figure S8: *Graphene sheet of 4 x 4 supercell doped with single N atom (a) along with the corresponding band structure graph (b)*

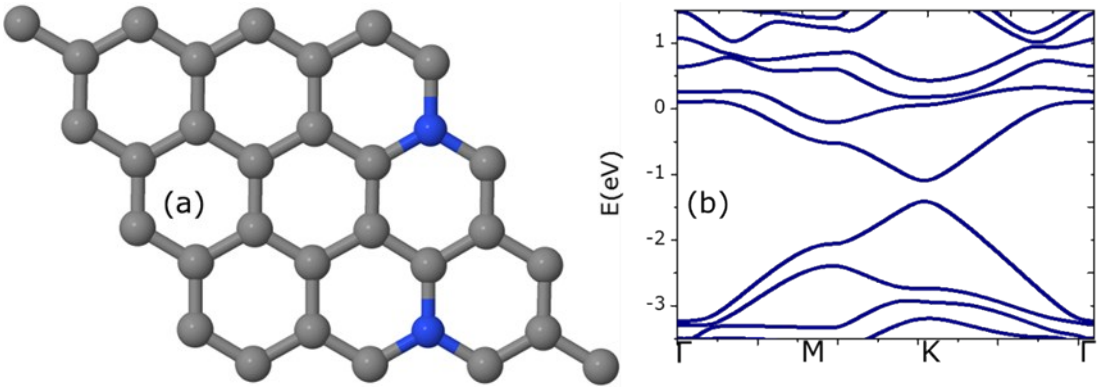

Figure S9: *Two N atoms doped in graphene sheet (rectangular configuration) is depicted in (a). The band structure graph is drawn in (b)*

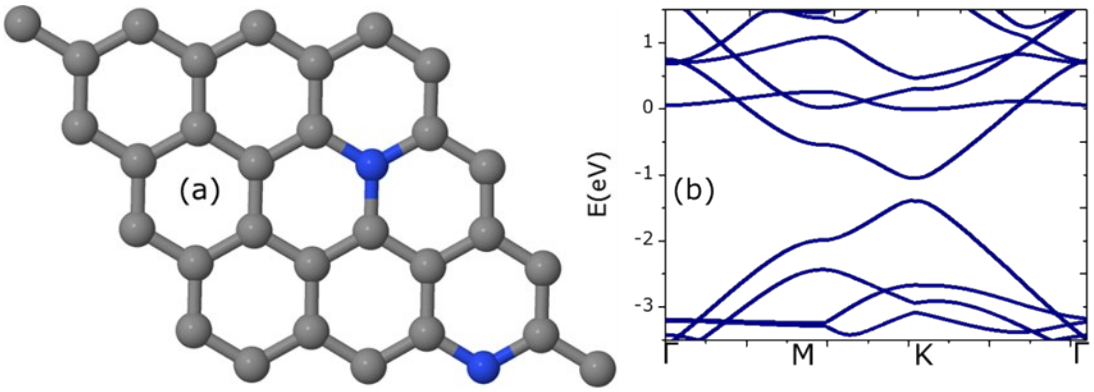

Figure S10: *Two N atoms doped in graphene sheet (hexagonal configuration) is depicted in (a). The band structure graph is drawn in (b)*

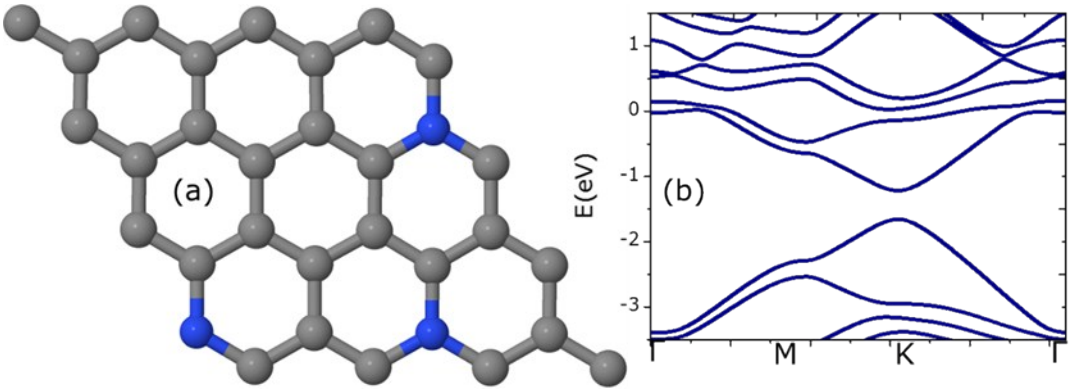

Figure S11: *Optimized geometry of graphene sheet doped with three N atom at rectangular sites (a) along with the corresponding band structure graph (b)*

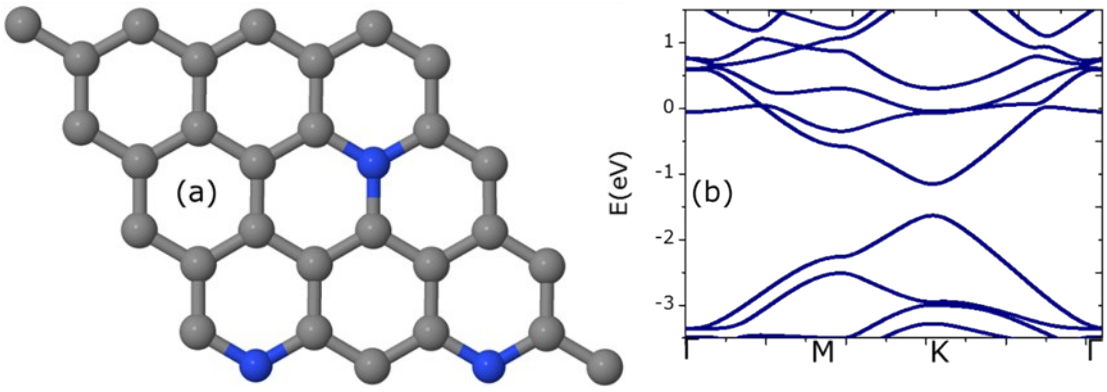

Figure S12: *Optimized geometry of graphene sheet doped with three N atom at hexagonal sites (a) along with the corresponding band structure graph (b)*

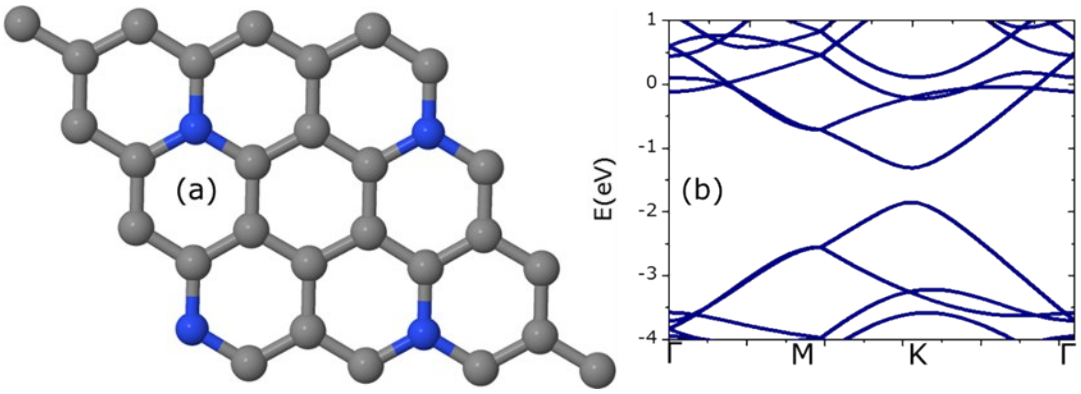

Figure S13: *Graphene sheet doped with four N atom at rectangular sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

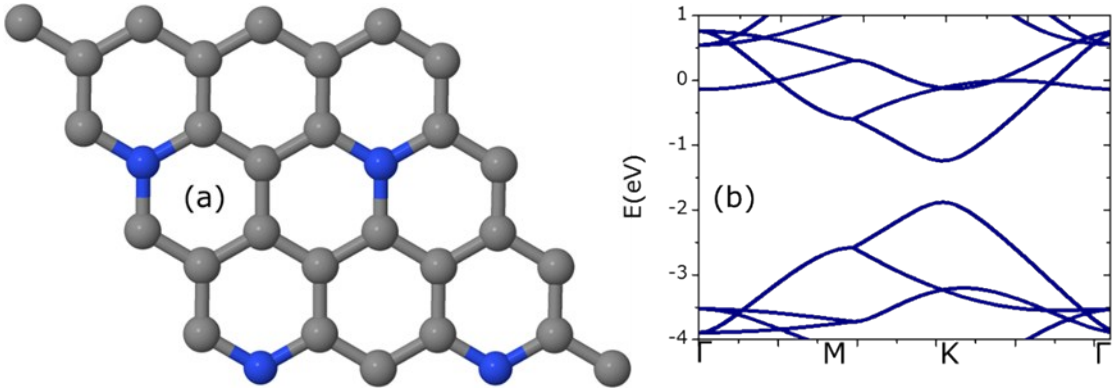

Figure S14: *Graphene sheet doped with four N atoms at hexagonal sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

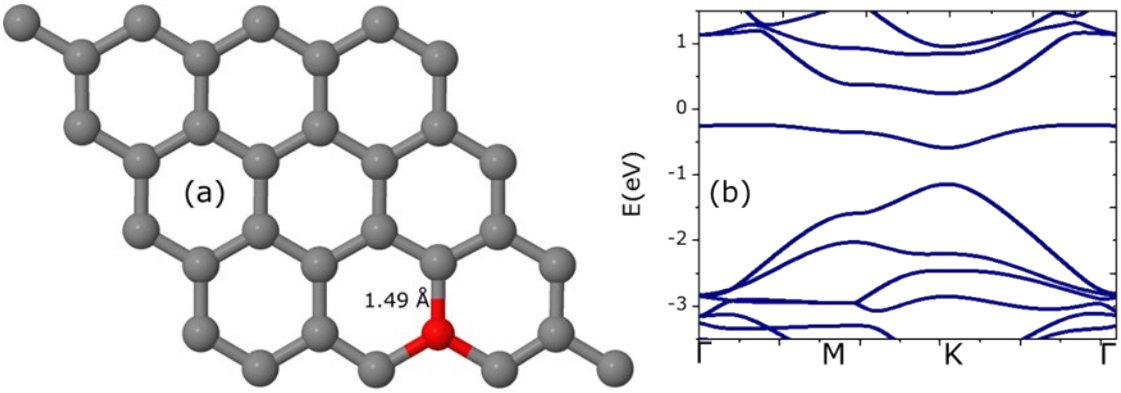

Figure S15: *Graphene sheet is doped with single O atom (a). The band structure calculated for this optimized geometry is drawn in (b)*

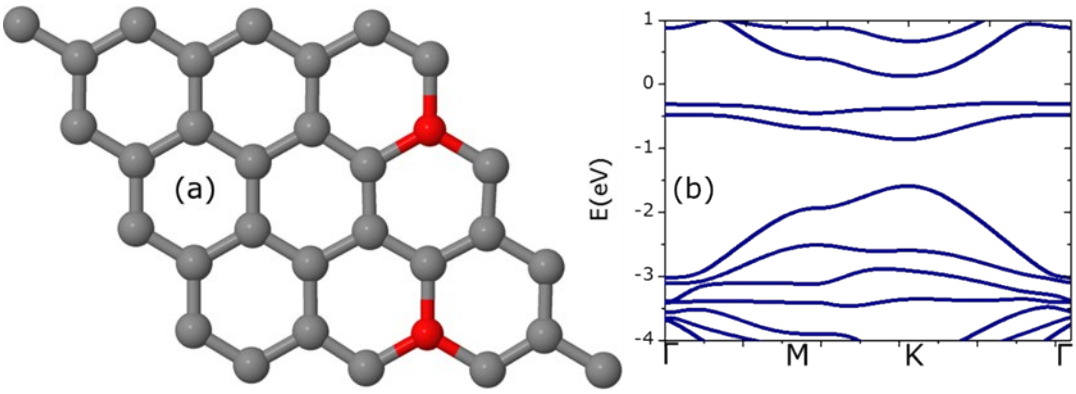

Figure S16: *Optimized geometry of graphene sheet doped with two O atoms at rectangular sites (a) along with the corresponding band structure graph (b)*

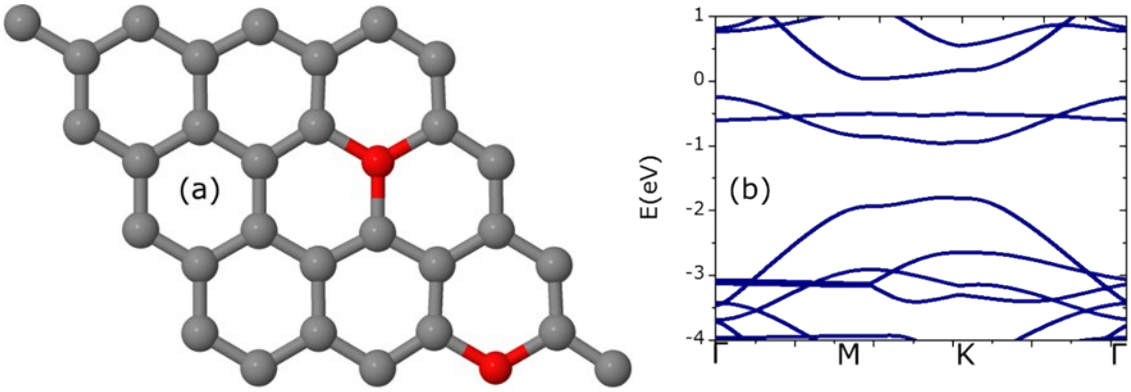

Figure S17: *Optimized geometry of graphene sheet doped with two O atoms at hexagonal sites (a) along with the corresponding band structure graph (b)*

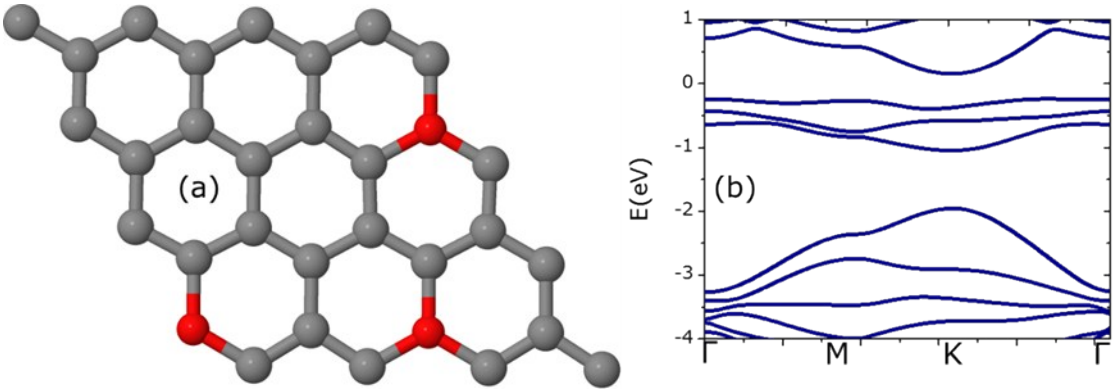

Figure S18: *Graphene sheet doped with three O atoms at rectangular sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

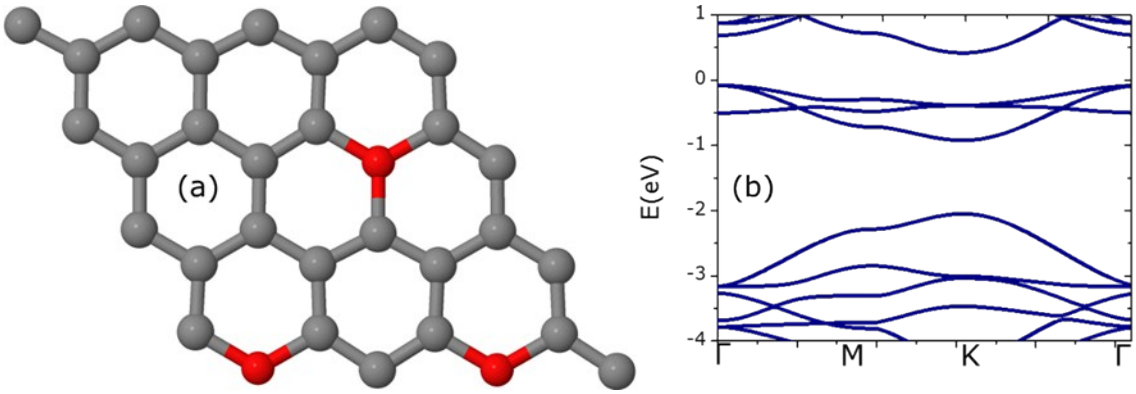

Figure S19: *Graphene sheet doped with three O atoms at hexagonal sites is shown in part (a) The band structure obtained from this system is shown in part (b)*

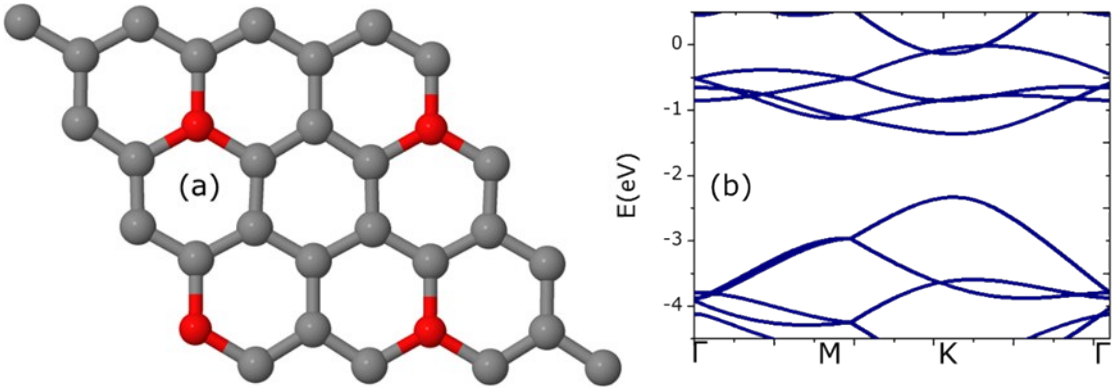

Figure S20: *Optimized geometry of graphene sheet doped with four O atoms at rectangular sites (a) along with the corresponding band structure graph (b)*

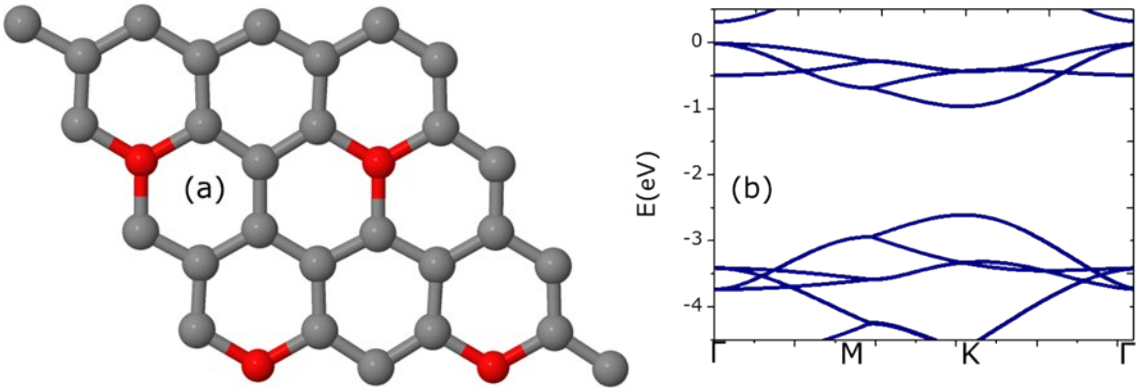

Figure S21: *Optimized geometry of graphene sheet doped with four O atoms at hexagonal sites (a) along with the corresponding band structure graph (b)*