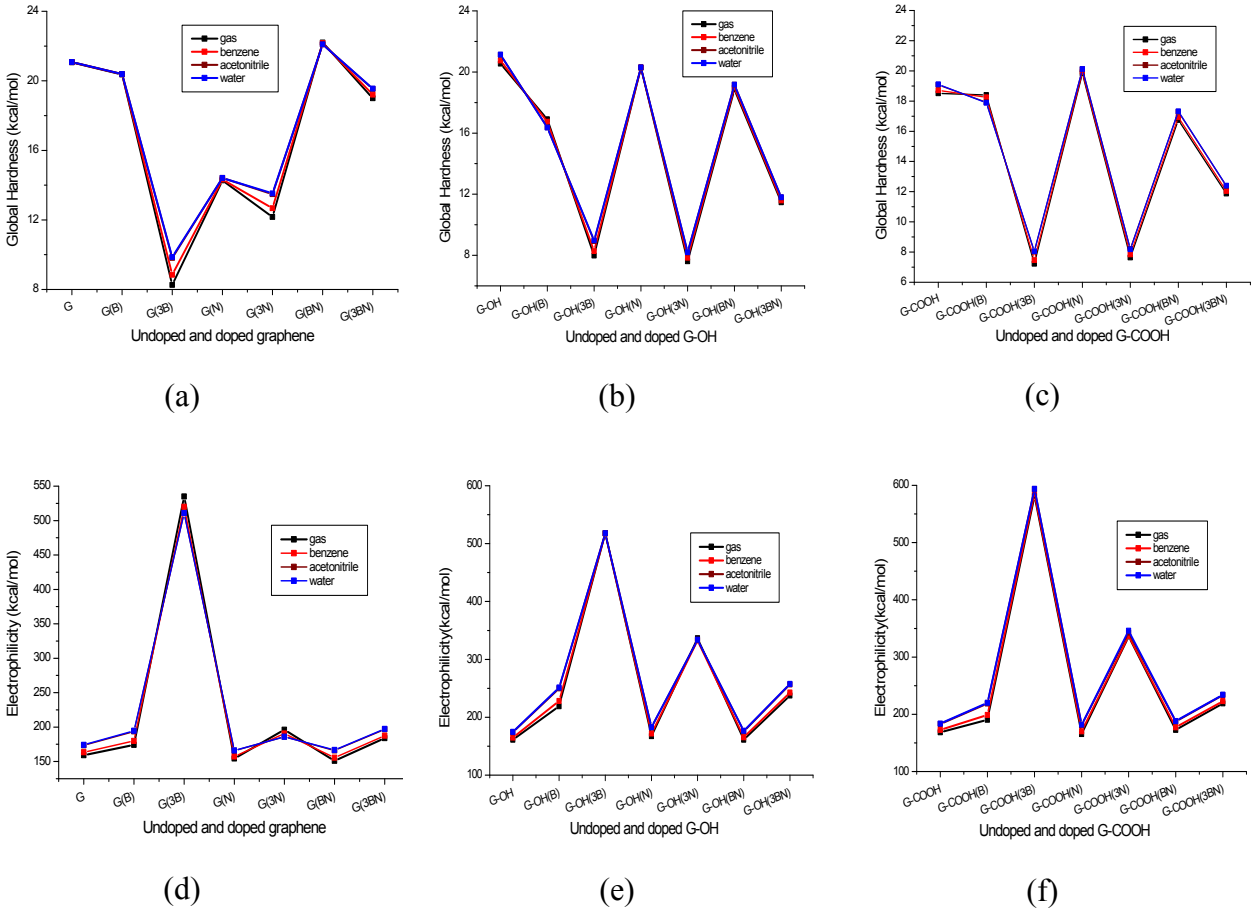
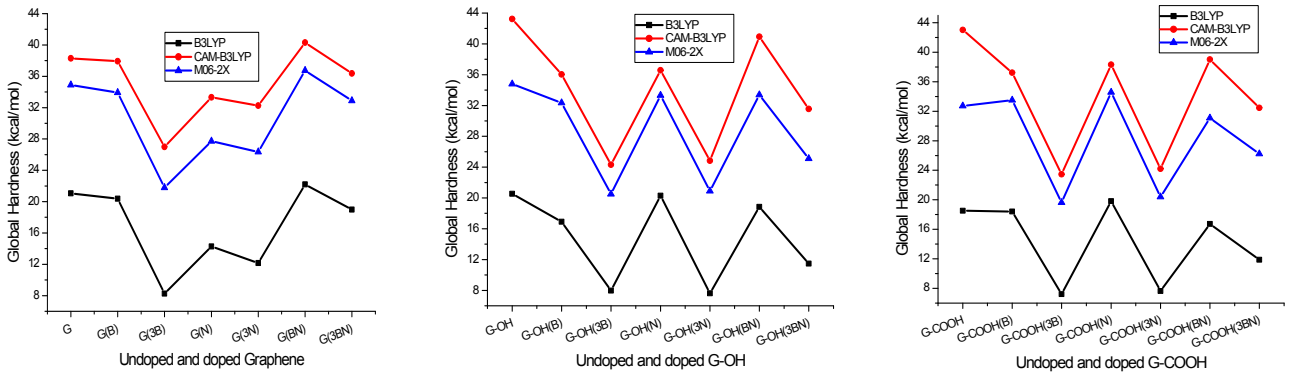
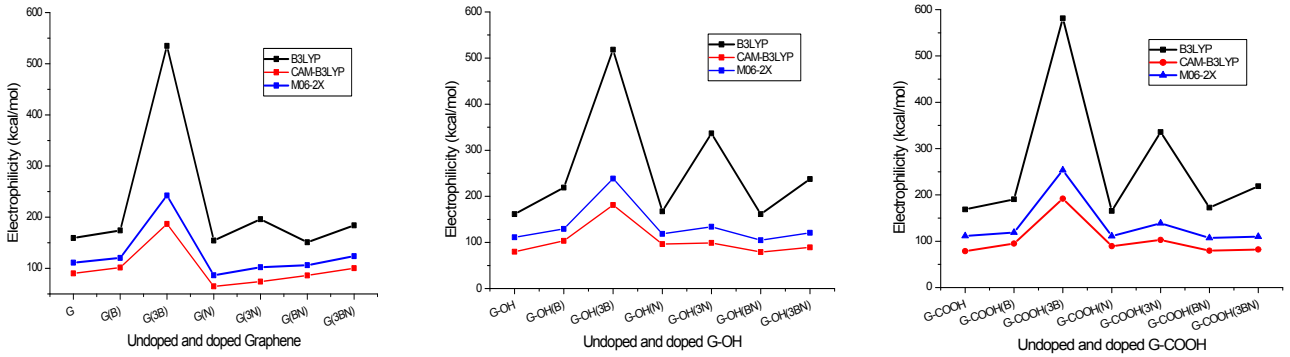
Electronic supplementary information



Supplementary Fig. S1 Variation in global hardness (a-c) and electrophilicity (d-f) of undoped and doped graphene, G–OH and G–COOH in gas and solvent phase at B3LYP/6-31G(d) level of theory

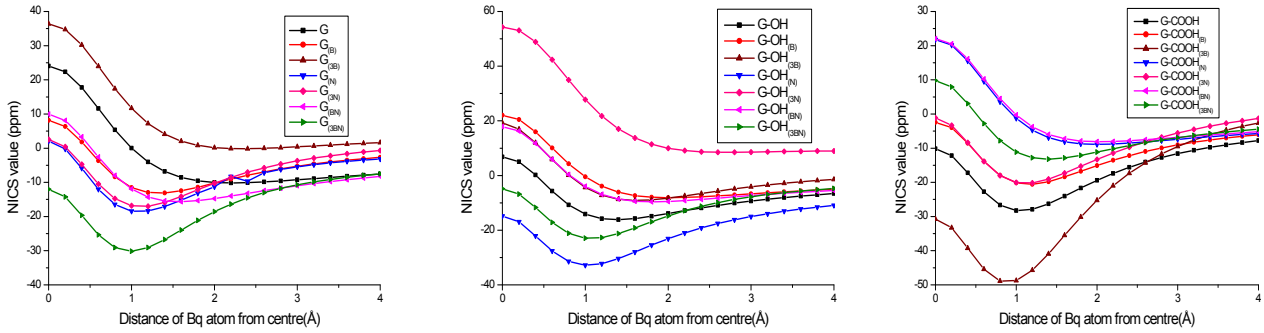


(a) (b) (c)



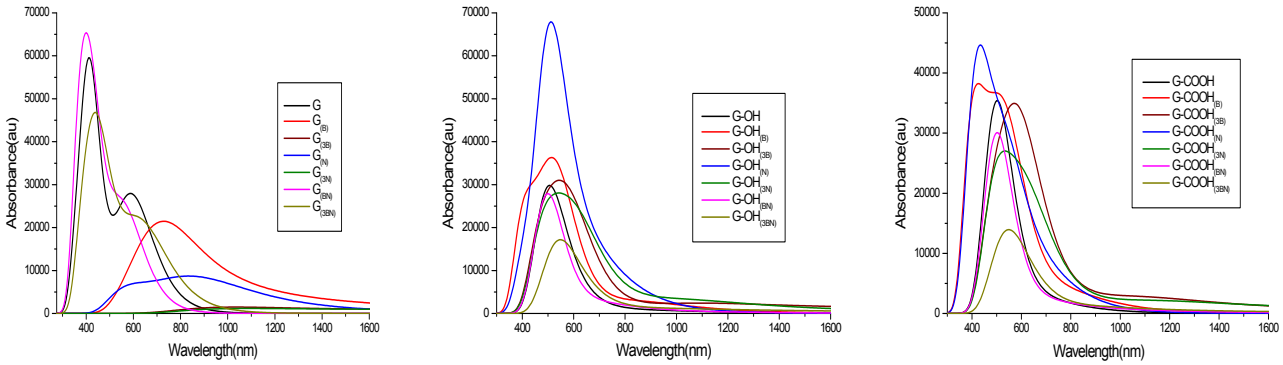
(d) (e) (f)

Supplementary Fig. S2 Variation in global hardness (a-c) and electrophilicity (d-f) of undoped and doped graphene, G–OH and G–COOH in gas phase using B3LYP, CAMB3LYP and M062X functional with 6-31G(d) basis set



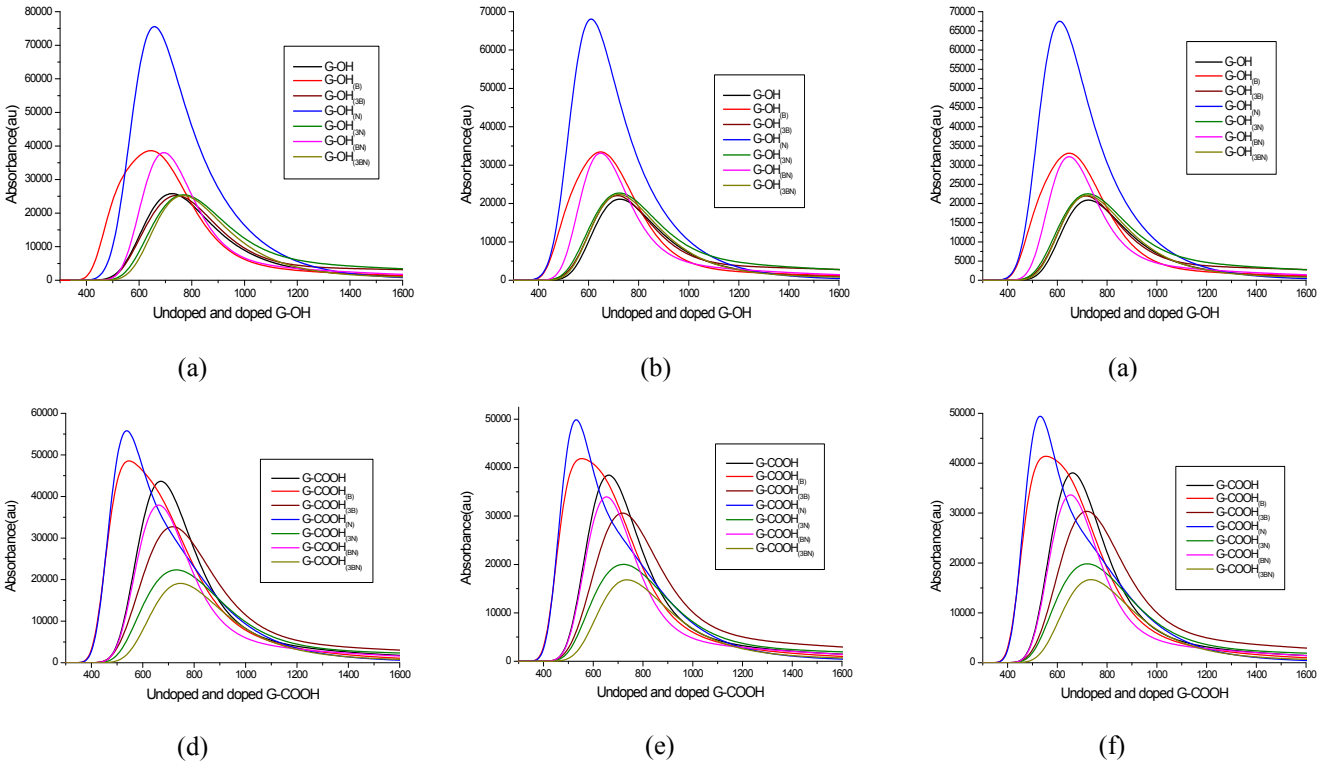
(a) (b) (c)

Supplementary Fig. S3 Variation in aromaticity ($NICS_{ZZ}$) at the edge of the undoped and doped (a) graphene (b) G–OH and (c) G–COOH at B3LYP/6-31G(d) level of theory.



(a) (b) (c)

Supplementary Fig. S4 UV-Visible absorption spectra of undoped and doped (a) graphene, (b) G–OH and (c) G–COOH in gas phase at CAM-B3LYP/6-31G(d) level of theory



Supplementary Fig. S5 UV-Visible absorption spectra of undoped and doped G–OH in (a) benzene (ε=2.27) (b) acetontrile (ε=35.69) (c) water (ε=78.35) and G–COOH in (d) benzene (ε=2.27) (e) acetontrile (ε=35.69) (f) water (ε=78.35) at B3LYP/6-31G(d) level of theory