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

Supporting Information

Mechanical properties and electronic structure of edge doped graphene nanoribbons with F, O and Cl atoms

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With the purpose to analyze the differences arising by the utilization of different xc-functionals here we present the comparison for X=F, O and Cl for N=4. We proceed with further DFT calculations, utilizing hybrid HSE06 functional[1]. For that reason, we utilized the VASP code[2-5] utilizing PAW-PBE[6] pseudopotentials with the same electronic configuration for the SIESTA setup.

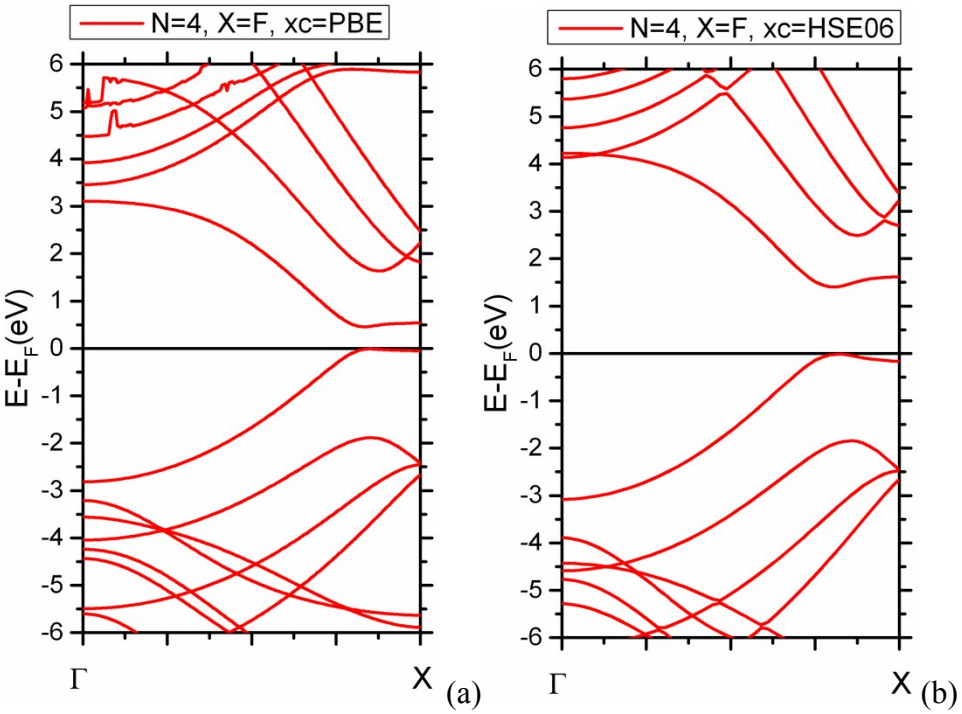

Figure S1.- Band Structure for X=F and N=4 utilizing GGA-PBE (a) and HSE06 (b)

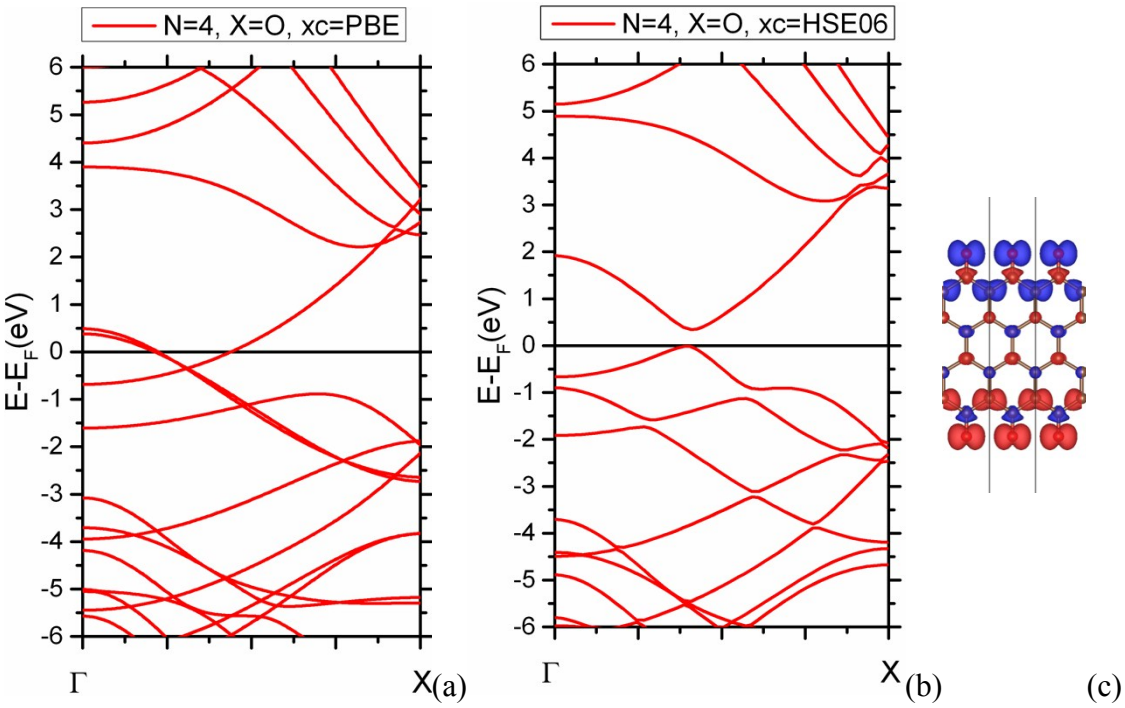

Figure S2.- Band Structure for X=O and N=4 utilizing GGA-PBE (a) and HSE06 (b) and the corresponding spin-density map (isosurface at 2E-3eÅ^{-3}) for HSE06 (c)

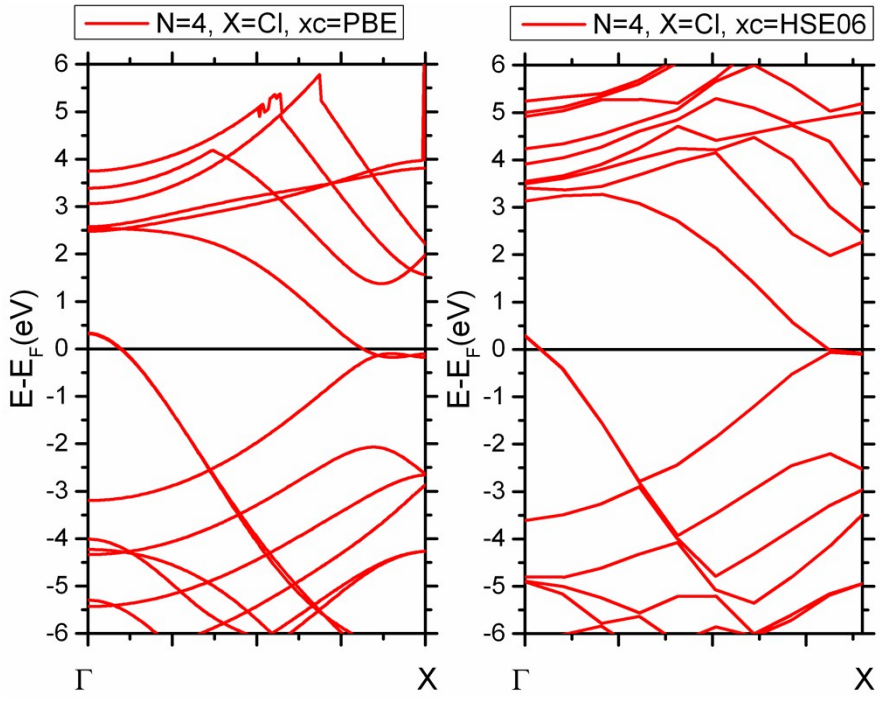

Figure S3.- Band Structure for X=Cl and N=4 utilizing GGA-PBE (a) and HSE06 (b)

References

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