Electronic Supplementary Material (ESI) for RSC Advances

SUPPORTING INFORMATION

This supporting information file contains the band structures and density of states figures for all the nanocarbon-halogen complexes considered in this study.

Figure S1: Electronic band structure of (a) Pristine graphene (b) Br_2 adsorbed graphene (c) I_2 adsorbed graphene (d) IBr adsorbed graphene (e) ICl adsorbed graphene; Electronic DOS of (a') Pristine graphene (b') Br_2 adsorbed graphene (c') I_2 adsorbed graphene (d') IBr adsorbed graphene (e') ICl adsorbed graphene. Fermi energy (E_F) is set to 0 eV

Figure S2: Electronic band structure of (a) Pristine CNT (5, 5) (b) Br_2 adsorbed CNT (5, 5) (c) I_2 adsorbed CNT (5, 5) (d) IBr adsorbed CNT (5, 5) (e) ICl adsorbed CNT (5, 5); Electronic DOS of (a') Pristine CNT (5, 5) (b') Br_2 adsorbed CNT (5, 5) (c') I_2 adsorbed CNT (5, 5) (d') IBr adsorbed CNT (5, 5) (e') ICl adsorbed CNT (5, 5). Fermi energy (E_F) is set to 0 eV

Figure S3: Electronic band structure of (a) Pristine CNT (8, 0) (b) Br_2 adsorbed CNT (8, 0) (c) I_2 adsorbed CNT (8, 0) (d) IBr adsorbed CNT (8, 0) (e) ICl adsorbed CNT (8, 0); Electronic DOS of (a') Pristine CNT (8, 0) (b') Br_2 adsorbed CNT (8, 0) (c') I_2 adsorbed CNT (8, 0) (d') IBr adsorbed CNT (8, 0) (e') ICl adsorbed CNT (8, 0). Fermi energy (E_F) is set to 0 eV.

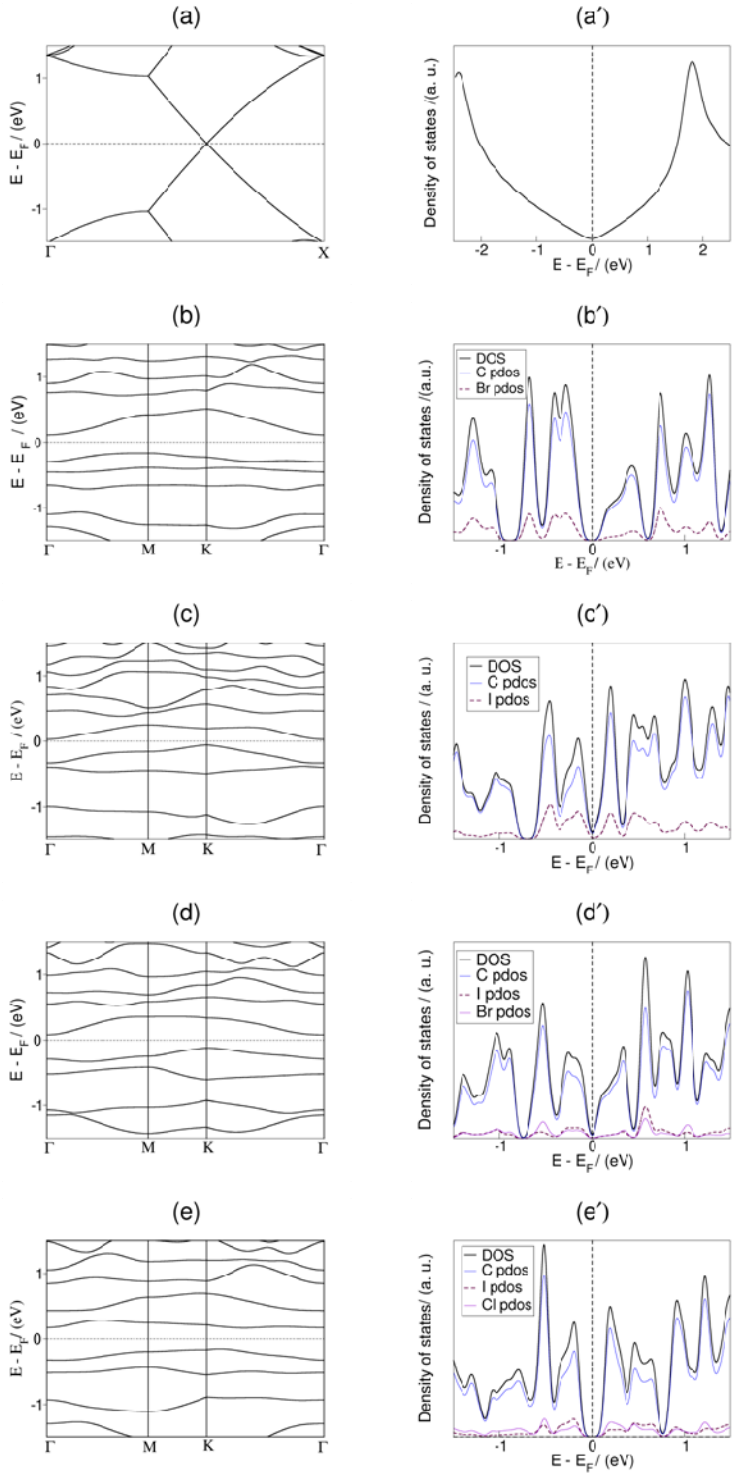

Figure S1

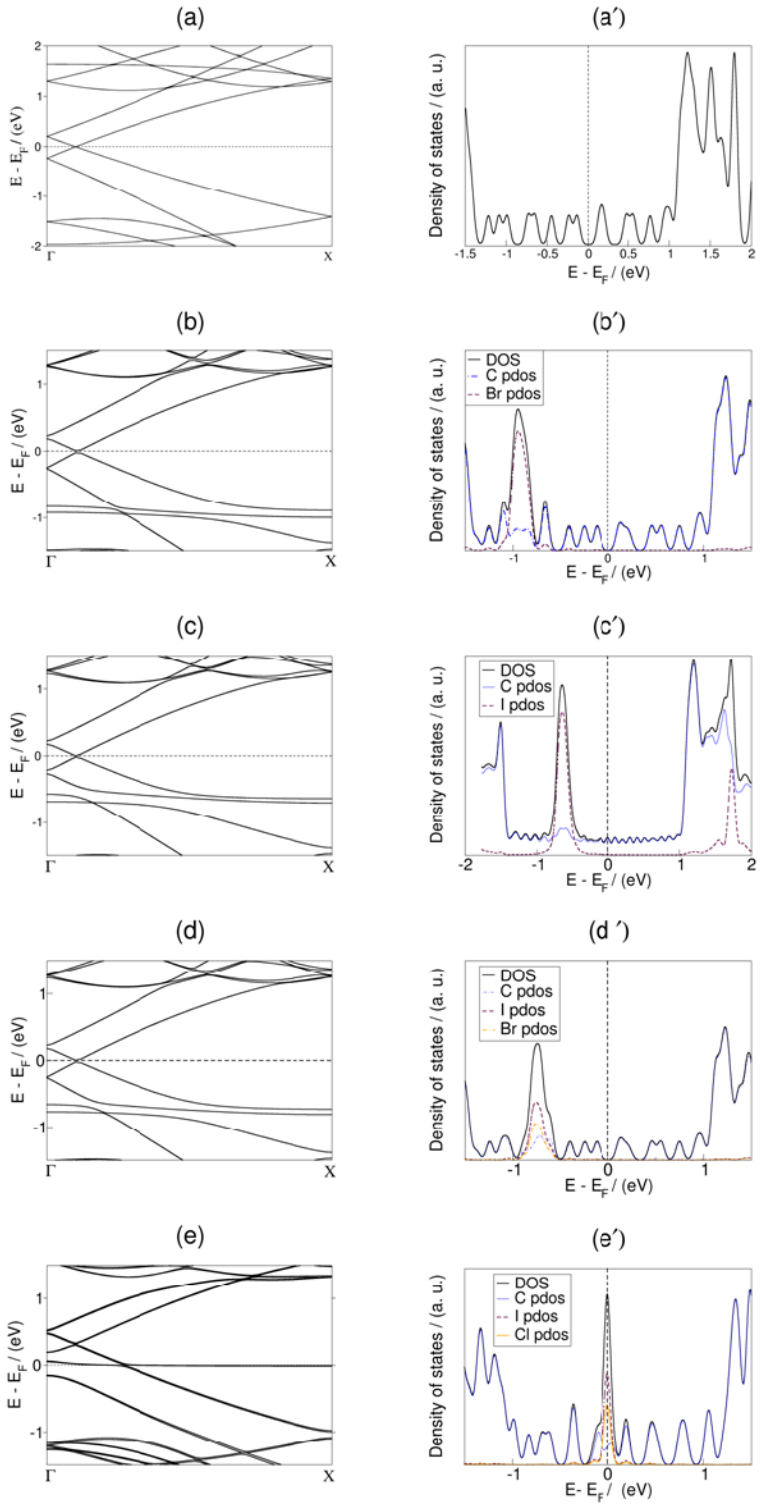

Figure S2

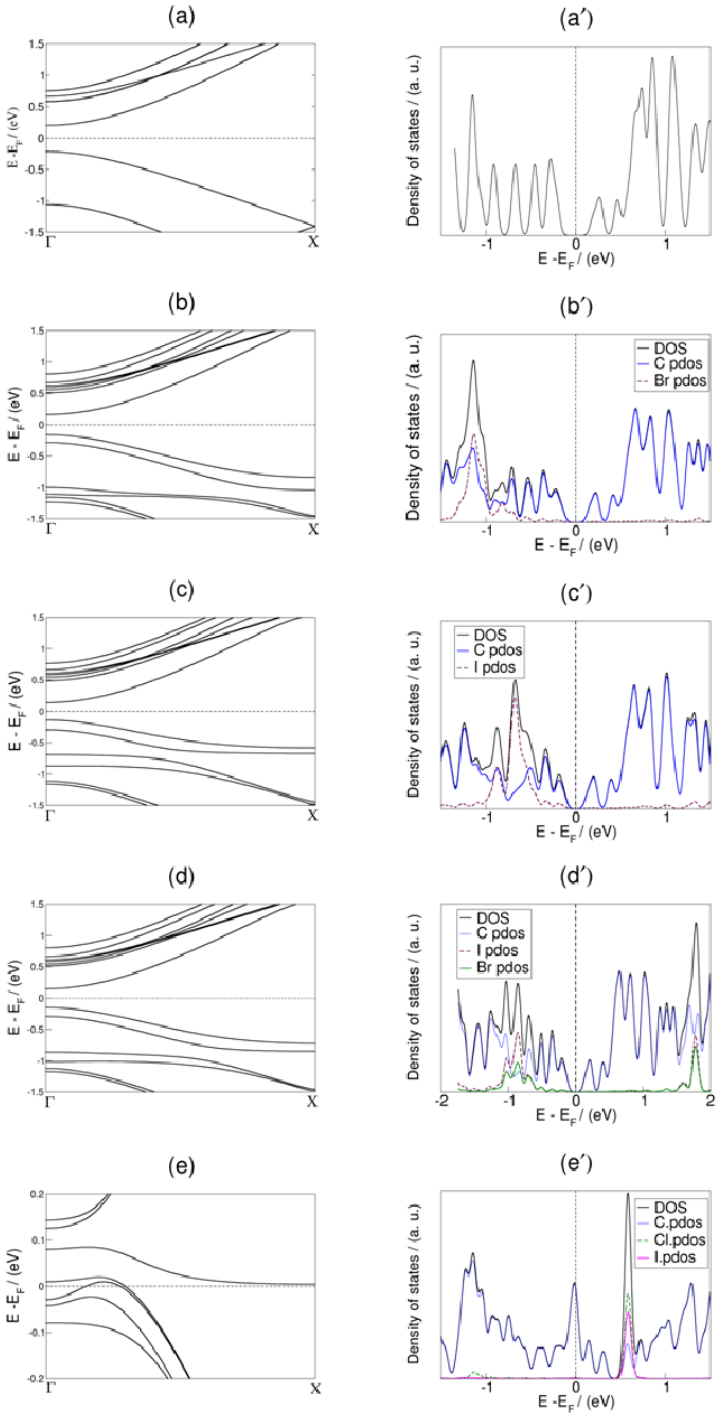

Figure S3