# Supporting Information

# Tune the chemical activity of graphene via the transition metal substrate

Yuan Ma[a], Lei Gao[a*], Yu Yan[a], Yanjing Su[a], and Lijie Qiao[a]

[a] Corrosion and Protection Center, Key Laboratory for Environmental Fracture (MOE), University of Science and Technology Beijing, Beijing 100083, China

Corresponding author: gaolei@ustb.edu.cn

## DOS prior to and after the adsorption of H or F atom

The density of states prior to and after the adsorption of H or F atom on the graphene/Re(0001) and graphene/Pt(111) are presented in Fig. S1. Here, one of the three nearest neighbor C atoms around the adsorption site and the substrate Re (or Pt) atom beneath were selected to calculate the partial density of states (PDOSs) of C atom $2p_z$ orbital and Re (or Pt) atom $5d_{z^2}$ orbital. The calculated PDOSs confirm the variations of charge transfer between the C atoms and substrate metal atoms after the adsorption of H or F atom.

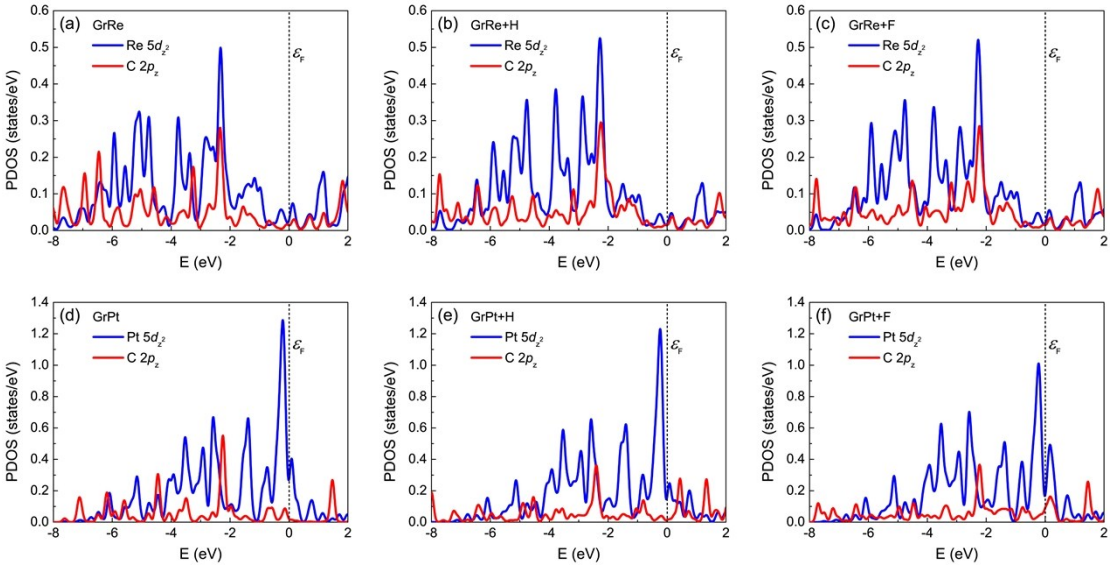


**Fig. S1** (a)-(c) The PDOSs of C atom $2p_z$ and Re atom $5d_{z^2}$ orbitals prior to and after the adsorption of H or F atom. (d)-(f) The PDOSs of C atom $2p_z$ and Pt atom $5d_{z^2}$ orbitals prior to and after the adsorption of H or F atom.