SUPPORTING INFORMATION FIGURES





HOMO AND LUMO OF P-Gr/H



HOMO AND LUMO OF P-Gr/F



HOMO AND LUMO OF SW-Gr/H



HOMO AND LUMO OF SW-Gr/F

Figure S1. Frontier Molecular Orbital distribution of Bare sheets.



ADSORPTION OF CO₂

HOMO AND LUMO OF P-Gr/F with CO₂



HOMO AND LUMO OF SW-Gr/H with CO₂



HOMO AND LUMO OF SW-Gr/F with CO₂

Figure S2. Frontier Molecular Orbital distribution of the most stable configurations of CO_2 adsorbed sheets.

ADSORPTION OF H₂O



HOMO AND LUMO OF P-Gr/H with H_2O



HOMO AND LUMO OF P-Gr/F with H_2O



HOMO AND LUMO OF SW-Gr/H with H_2O



HOMO AND LUMO OF SW-Gr/F with H₂O

Figure S3. Frontier Molecular Orbital distribution of the most stable configurations of H_2O adsorbed sheets.