

SUPPLEMENTARY INFORMATION

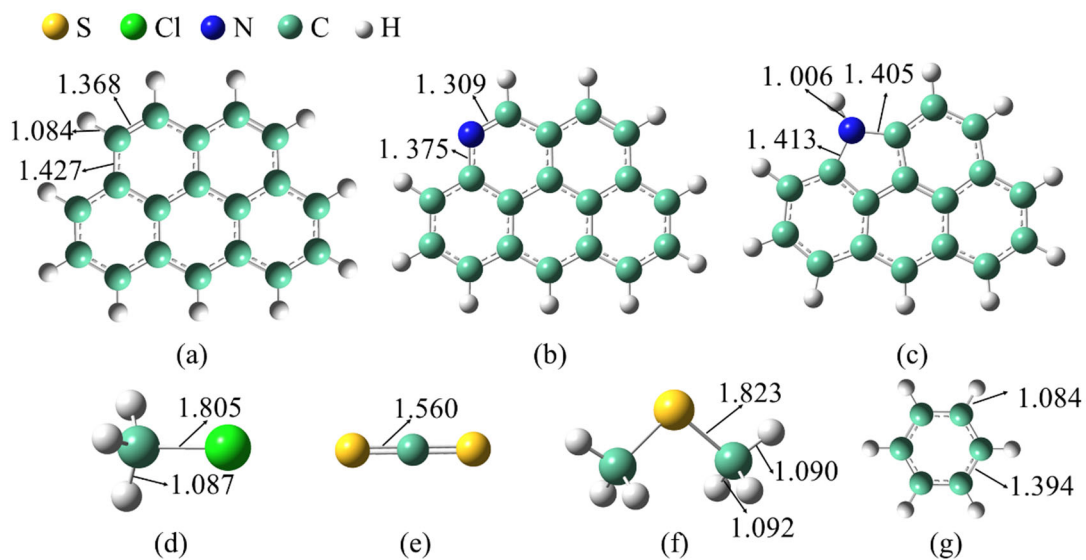


Figure S1. Molecular models of activated carbon and volatile organic compounds (VOCs): (a) NF, (b) PD, (c) PR, (d) CH₃Cl, (e) CS₂, (f) C₂H₆S, and (g) C₆H₆. Typical bond lengths (Å) have been marked with text.

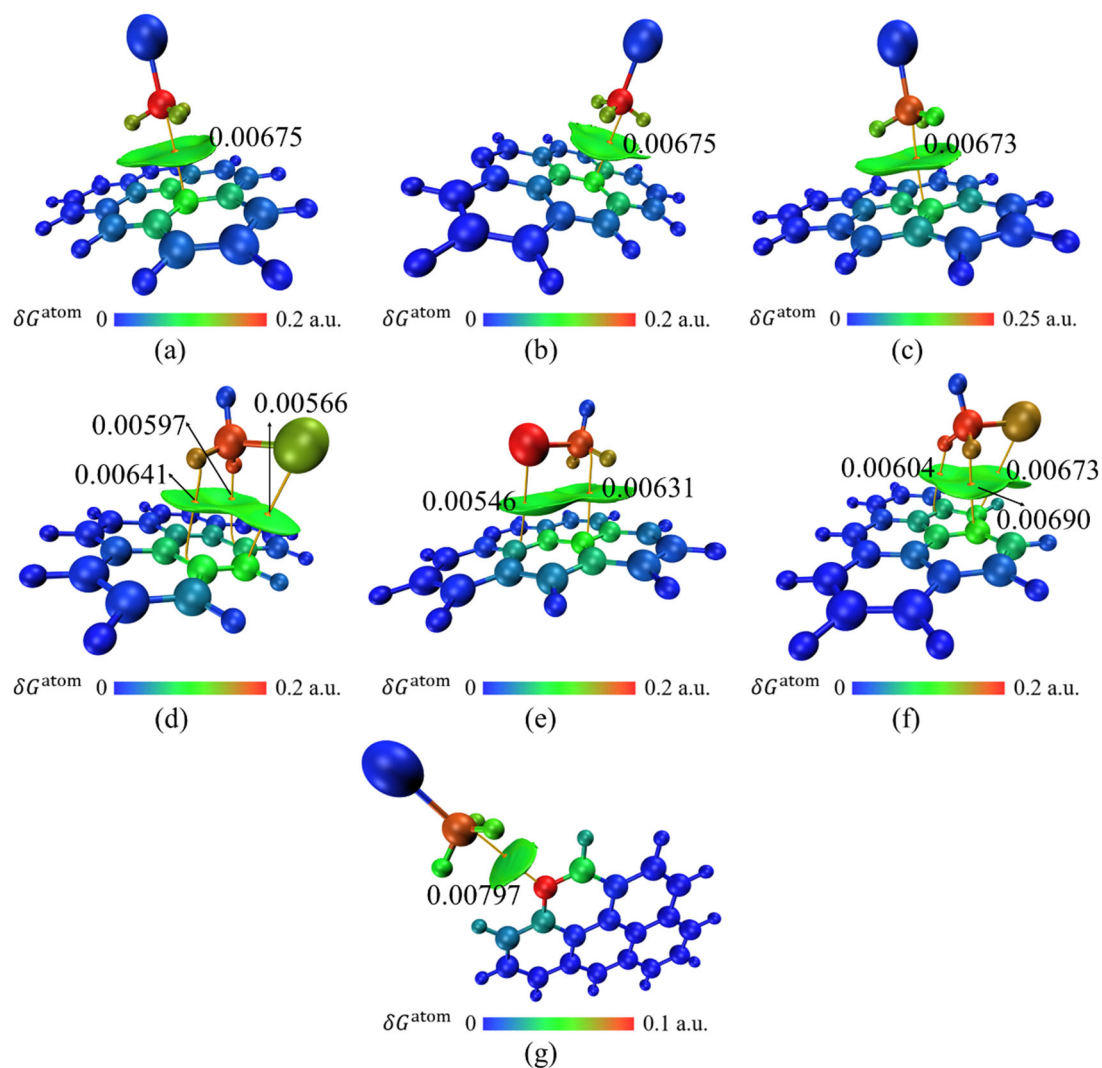


Figure S2. IGMH analysis diagram depicting the adsorption of CH_3Cl on different activated carbon surfaces: (a,d) NF plane, (b,e) PD plane, (c,f) PR plane, and (g) PD edge. Atoms are colored by δG^{atom} . Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts.

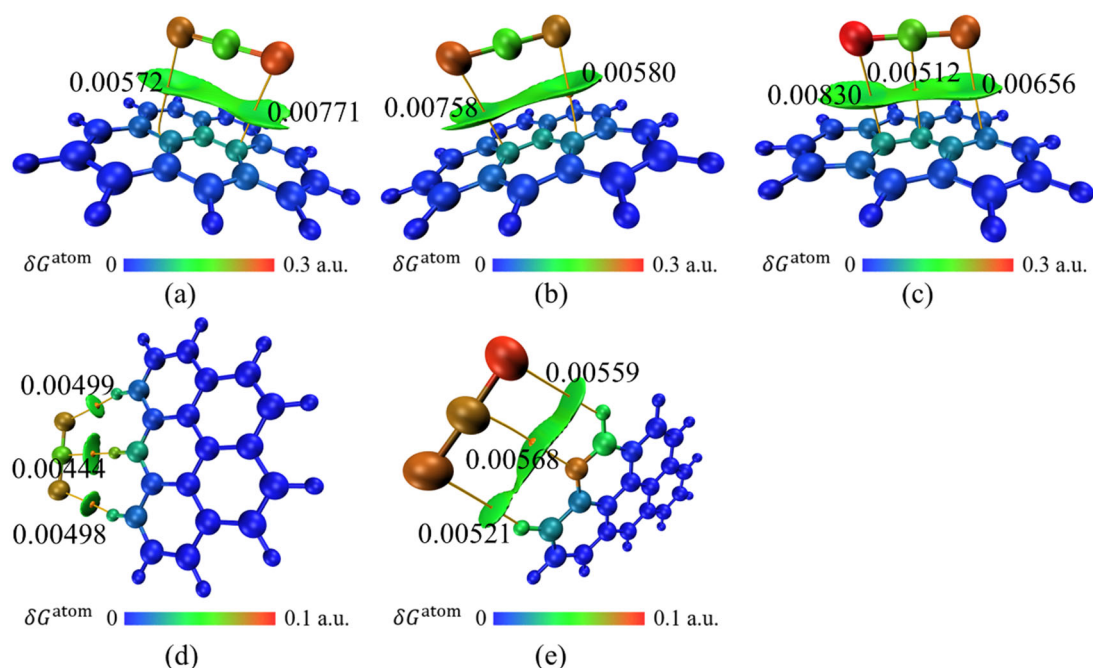


Figure S3. IGMH analysis diagram depicting the adsorption of CS_2 on different activated carbon surfaces: (a) NF plane, (b) PD plane, (c) PR plane, (d) NF edge, and (e) PD edge. Atoms are colored by δG^{atom} . Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts.

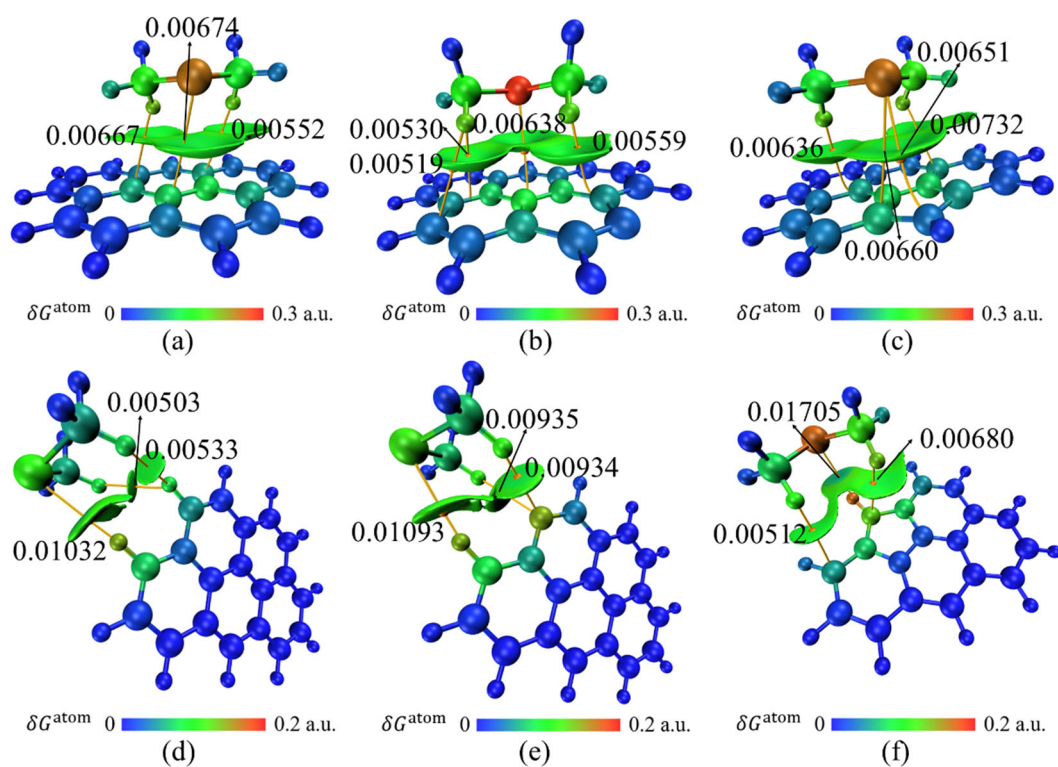


Figure S4. IGMH analysis diagram depicting the adsorption of $\text{C}_2\text{H}_6\text{S}$ on different activated carbon surfaces: (a) NF plane, (b) PD plane, (c) PR plane, (d) NF edge, and (e) PD edge. Atoms are colored by δG^{atom} . Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts.

activated carbon surfaces: **(a)** NF plane, **(b)** PD plane, **(c)** PR plane, **(d)** NF edge, **(e)** PD edge, and **(f)** PD edge. Atoms are colored by δG^{atom} . Bond critical points (orange spheres) and bond paths (brown lines) are also shown. Electron density values (a.u.) at the bond critical points are indicated by texts.