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Supplementary information for: "Disclosure of the Nano-scale Hydrogen Ballet on Mono-Vacancy Graphene: A Dance of Reactivity with Incoming Gases"

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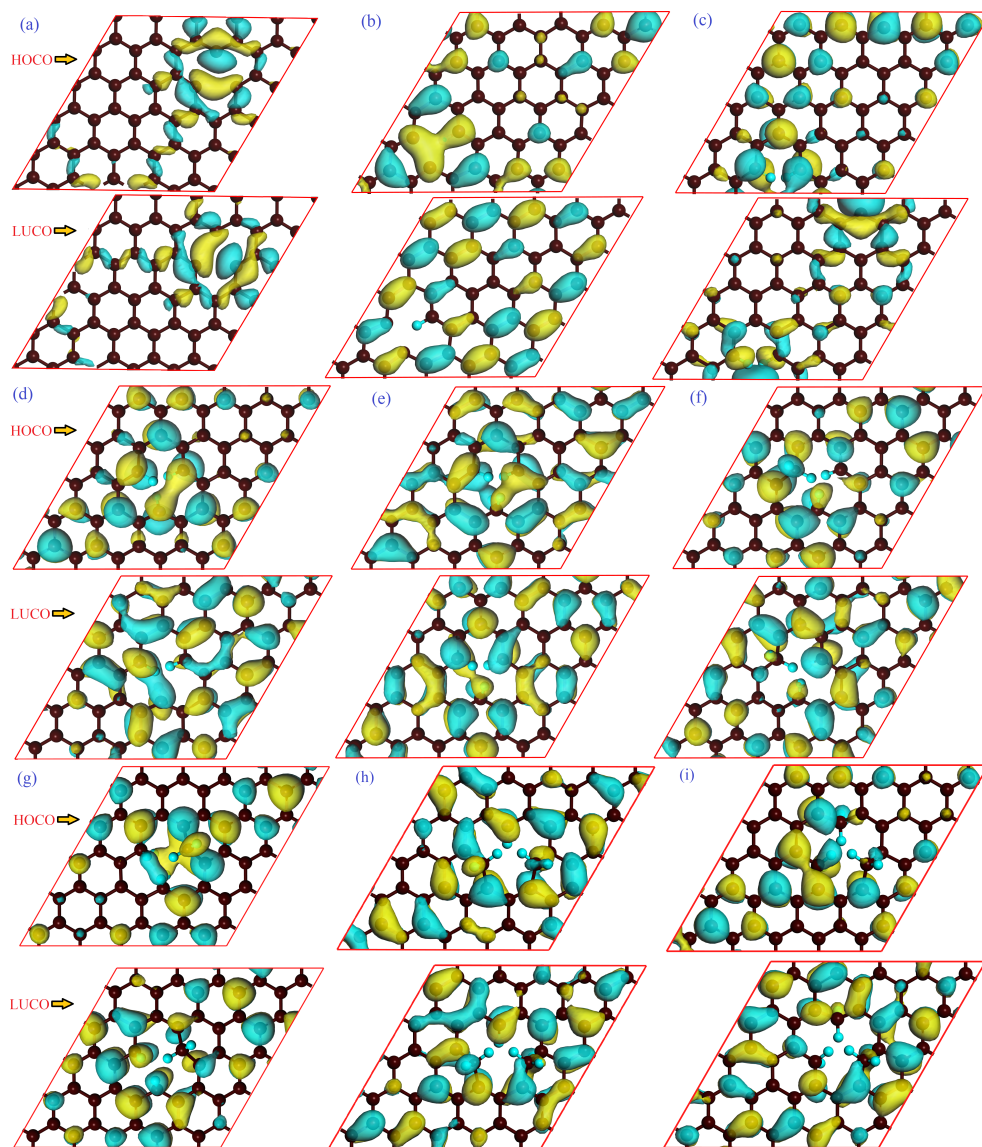


Fig.S 1 Top: the Highest Occupied Crystal Orbital (HOCO), and Bottom: Lowest Unoccupied Crystal Orbital (LUCO) of (a) monovacancy graphene, (b) hydrogenated monovacancy graphene (H_x -MVG, $x=1$), (c) H_2 -MVG, (d) H_3 -MVG, (e) H_4 -MVG, (f) H_5 -MVG, (g) H_6 -MVG, (h) $H_6(2)$ -MVG, and (i) H_7 -MVG.

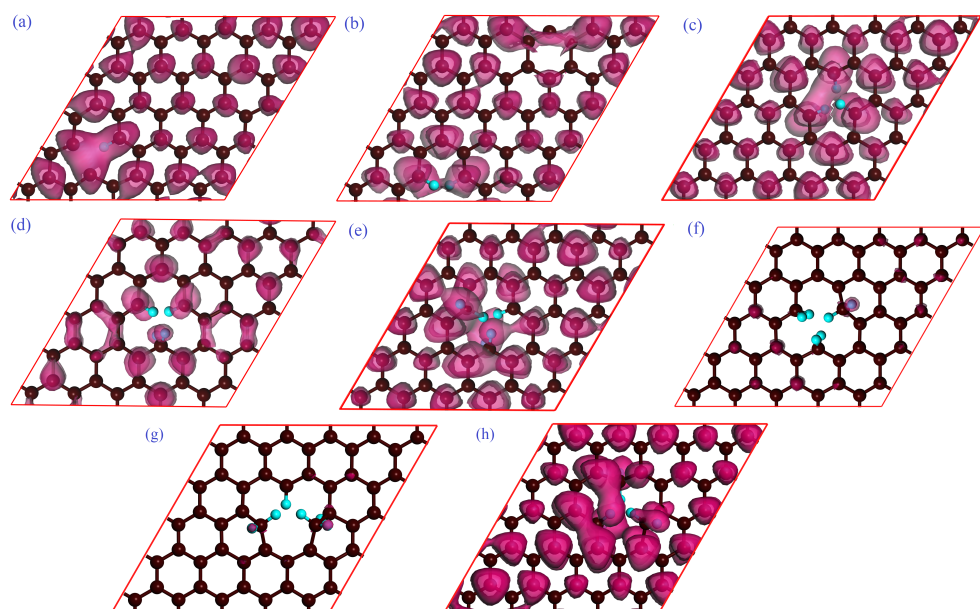


Fig S 2 The electrophilic Fukui function profile of (a) hydrogenated monovacancy graphene (H_x -MVG, $x=1$), (b) H_2 -MVG, (c) H_3 -MVG, (d) H_4 -MVG, (e) H_5 -MVG, (f) H_6 -MVG, (g) $H_6(2)$ -MVG, and (h) H_7 -MVG.

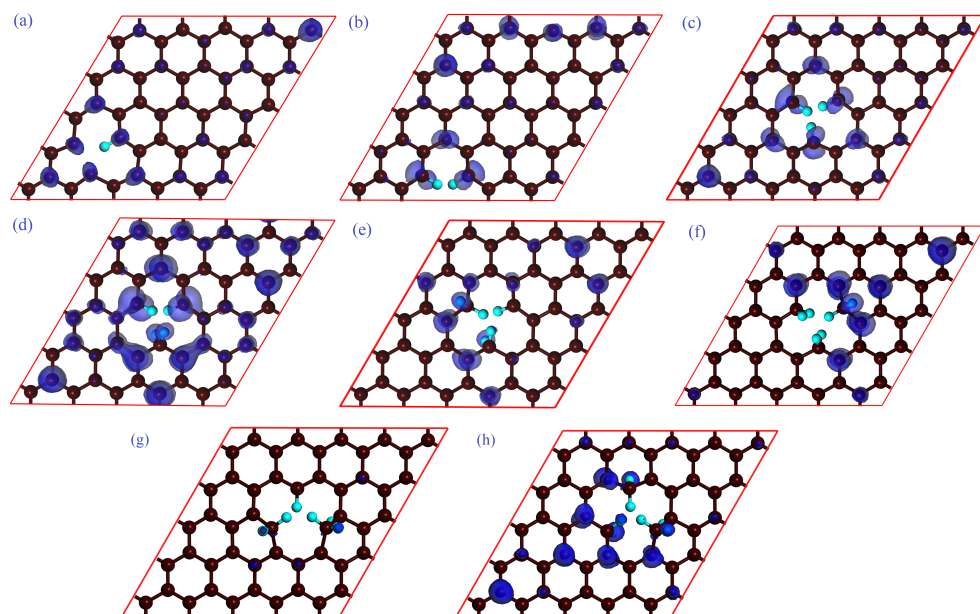


Fig S 3 The nucleophilic Fukui function profile of (a) hydrogenated monovacancy graphene (H_x -MVG, $x=1$), (b) H_2 -MVG, (c) H_3 -MVG, (d) H_4 -MVG, (e) H_5 -MVG, (f) H_6 -MVG, (g) $H_6(2)$ -MVG, and (h) H_7 -MVG.

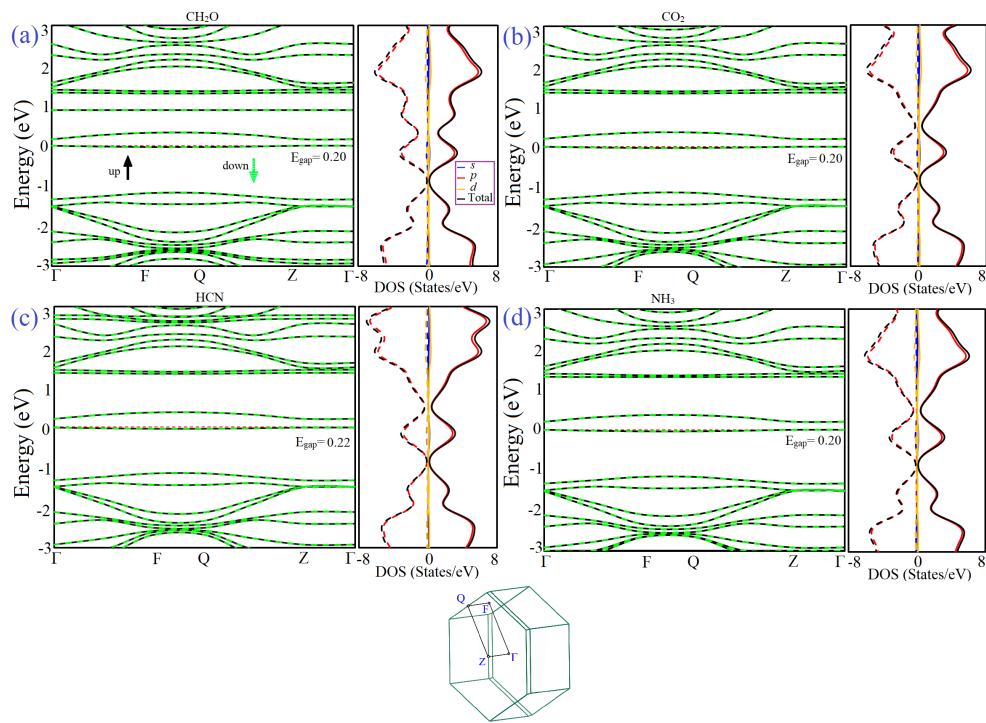


Fig.S 4 Left-hand side: The spin-unrestricted electronic band structure, Right-hand side: total density of states (TDOS), and partial density of states (PDOS) of adsorbed gases on H₆-MVG, (a) CH₂O, (b) CO₂, (c) HCN, and (d) NH₃. The electronic band gap (E_{gap} ; eV) is indicated in black within the electronic band structure. The zero of energy is at the Fermi level. The inset indicates the first Brillouin zone path.