

Density Functional Theory Analysis of the Impact of Boron Concentration and Surface Oxidation in Boron-Doped Graphene for Sodium and Aluminum Storage

Supplementary Information

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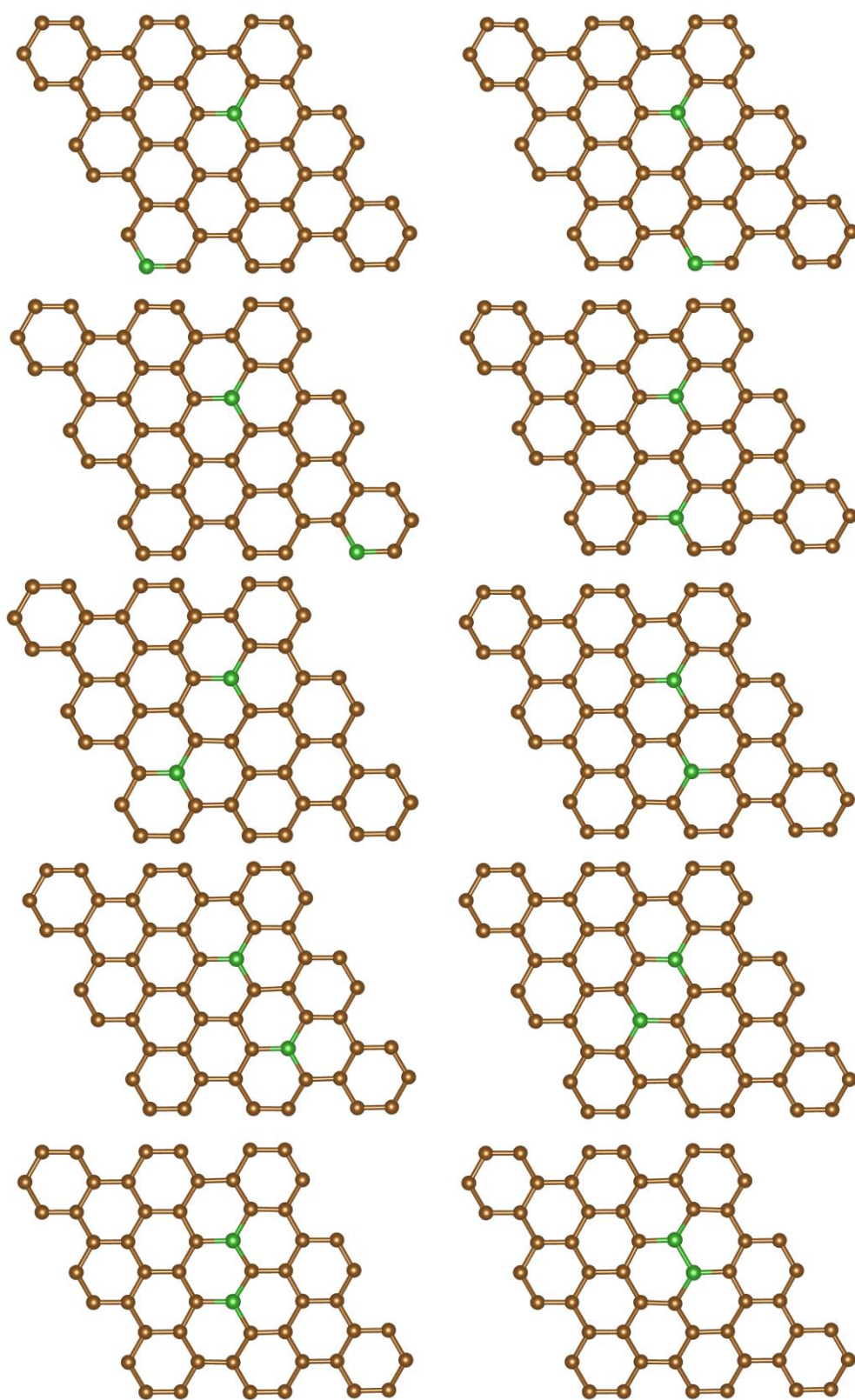


Figure S1. Investigated configurations of $C_{52}B_2$.

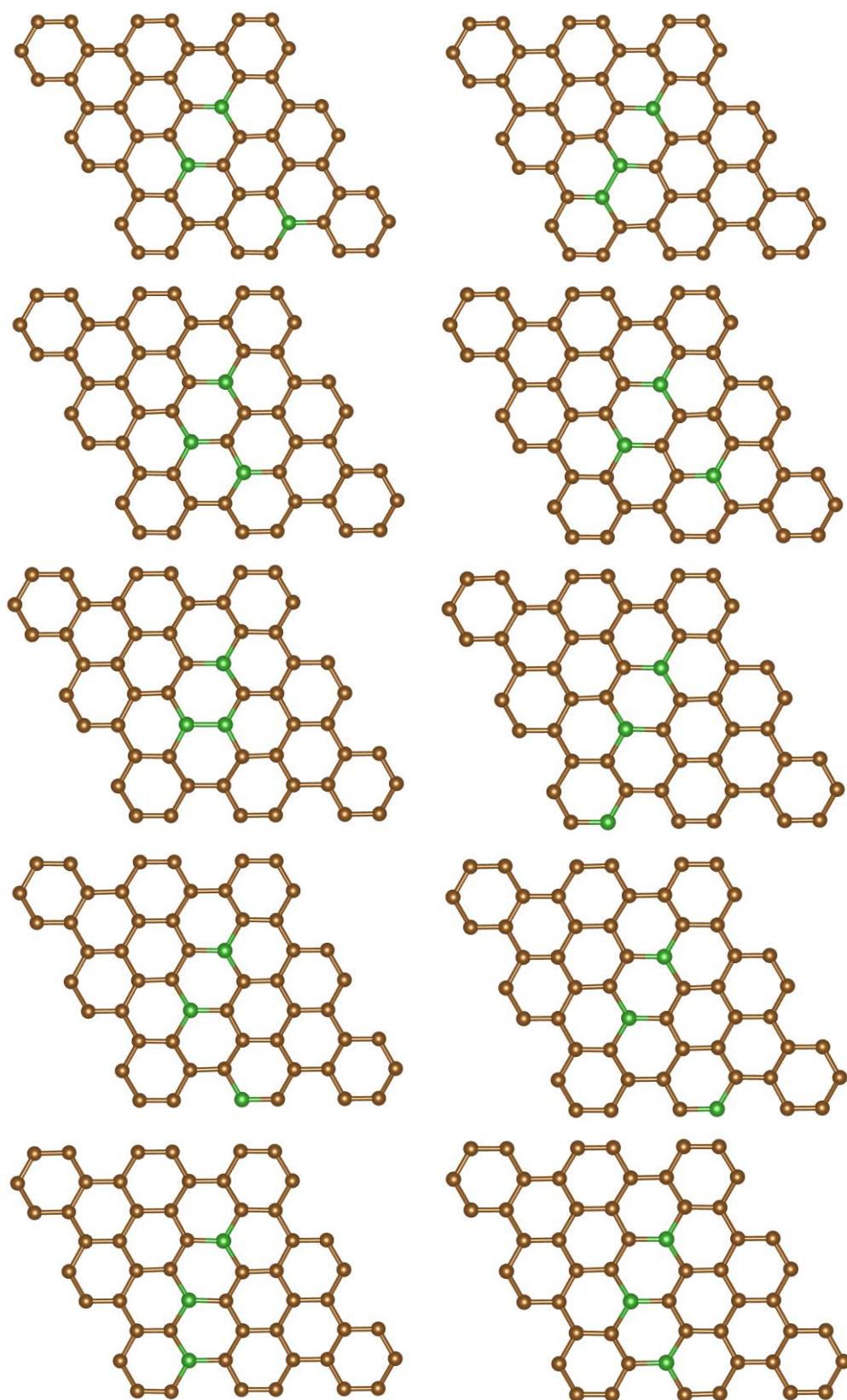


Figure S2. Investigated configurations of $C_{51}B_3$.

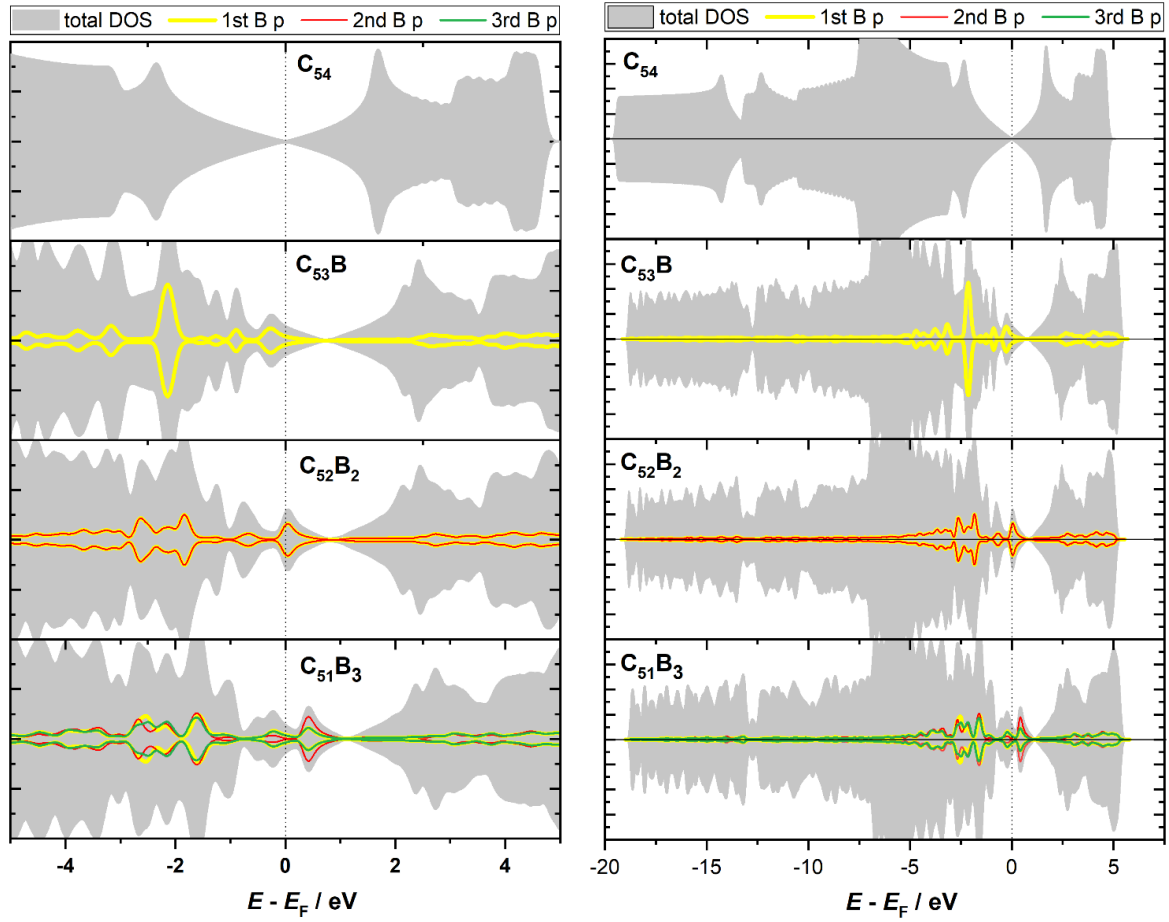


Fig. S3. Electronic structures (total DOS) of pristine graphene (C_{54} , first row) and investigated boron-doped graphenes $C_{54-n}B_n$ (bottom three rows), zoomed in to the range from -5 to $+5$ eV (left) and in full energy range (right). The p states of boron dopant atoms are shown separately (in case of $C_{52}B_2$, the p states of two B atoms overlap). For clarity, all total DOS plots are divided by 5. The Fermi level (dashed, black line) is set to 0.

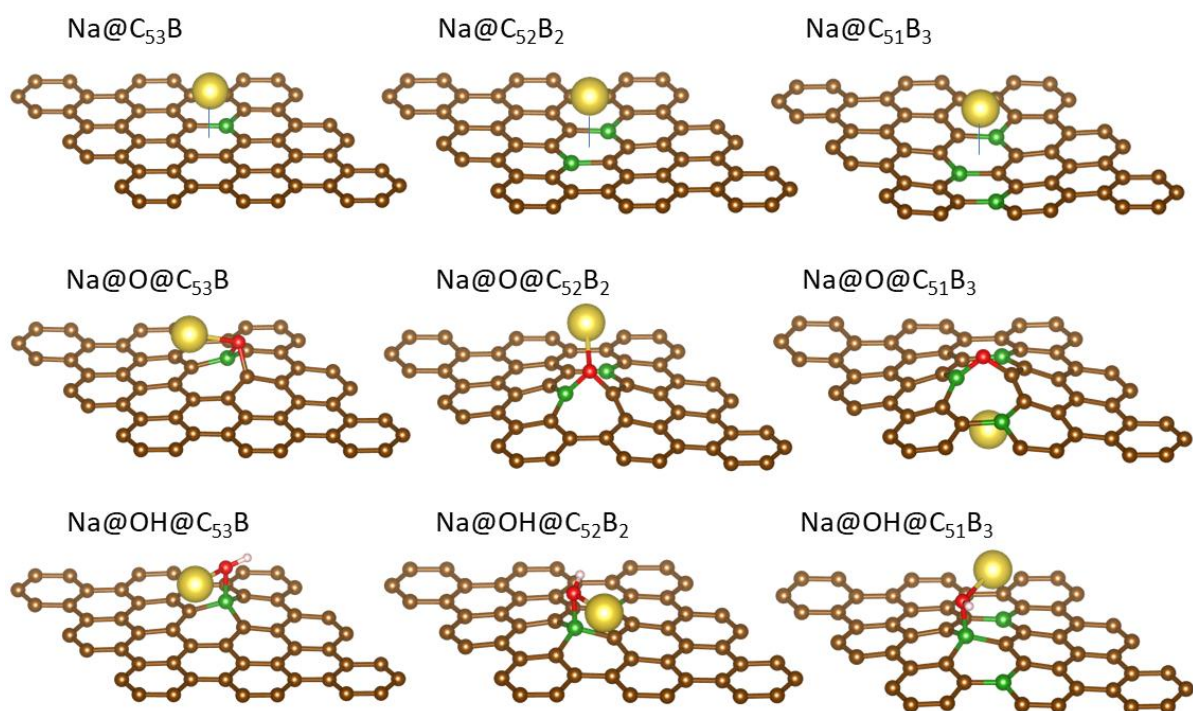


Fig. S4. Optimized structures of Na adsorption onto (oxidized) C_{54-n}B_n systems (first row: bare C_{54-n}B_n, middle row C_{54-n}B_n oxidized by O_{ads}, bottom row C_{54-n}B_n oxidized by OH_{ads}). Graphical representations was made using VESTA.

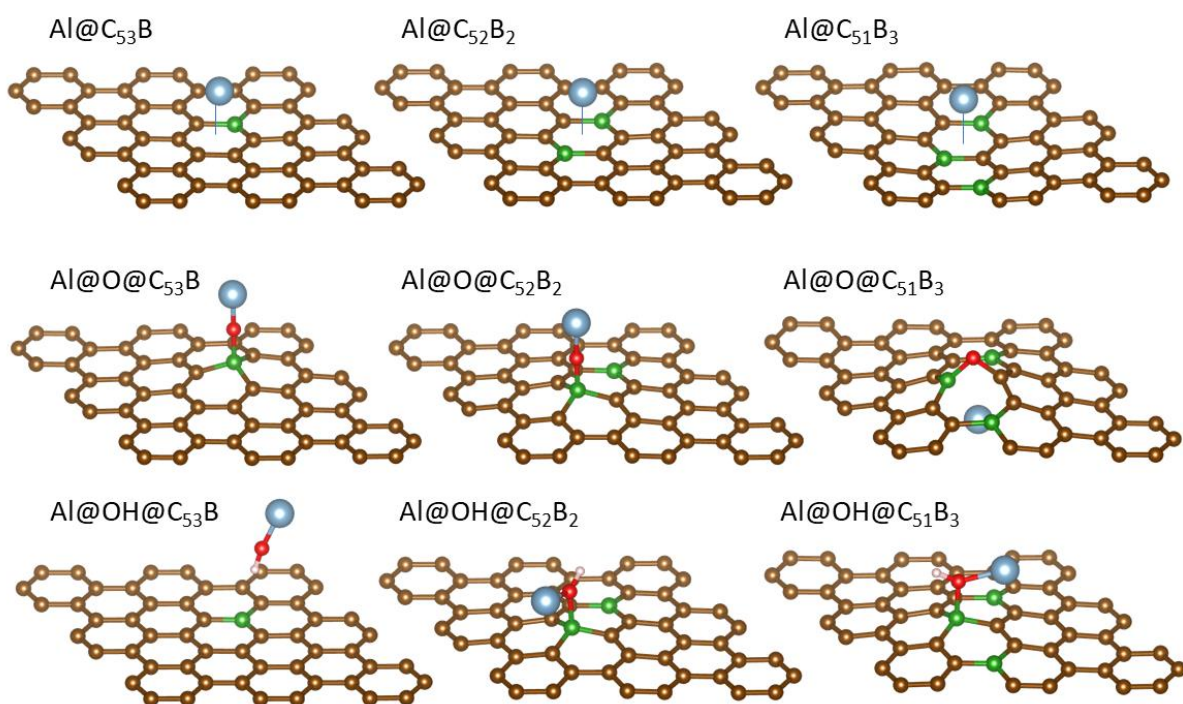


Fig. S5. Optimized structures of Al adsorption onto (oxidized) C_{54-n}B_n systems (first row: bare C_{54-n}B_n, middle row C_{54-n}B_n oxidized by O_{ads}, bottom row C_{54-n}B_n oxidized by OH_{ads}). Graphical representations were made using VESTA.