Supporting Information of

# Popgraphene: a new 2D Planar Carbon Allotrope Composed of 5−8−5 Carbon Rings for High-performance Lithium-ion Battery Anodes from Bottom-up Programming

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Figure S1. Band structures and density of states (DOS) of a popgraphene sheet based on the PBE functional and vdW corrections.

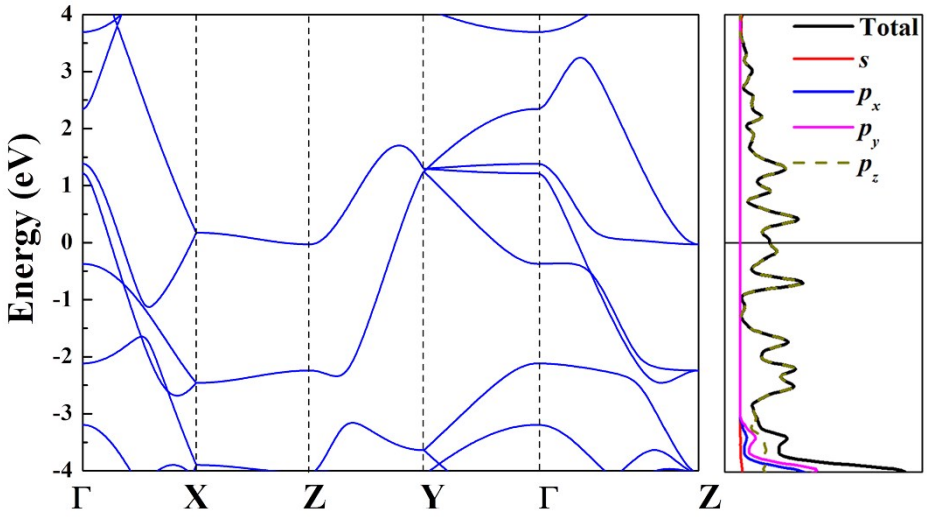

Figure S2. Band structures of a popgraphene sheet based on both HSE and PBE functionals without considering vdW corrections.

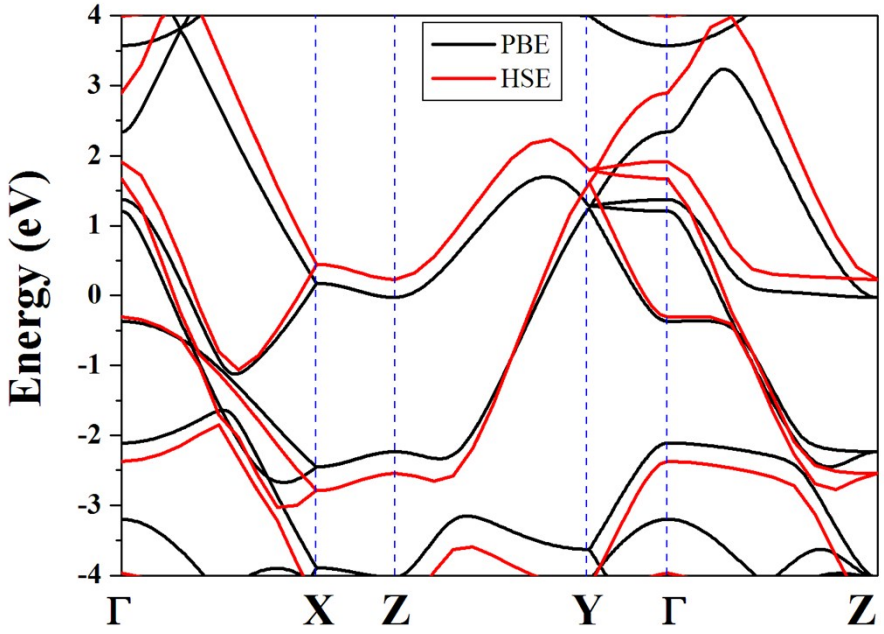

Figure S3. The band structures of a popgraphene sheet under uniaxial and biaxial loading at the strains of ±5% without vdW corrections. +5% occurs under tensile loading, whereas -5% happens under compression.

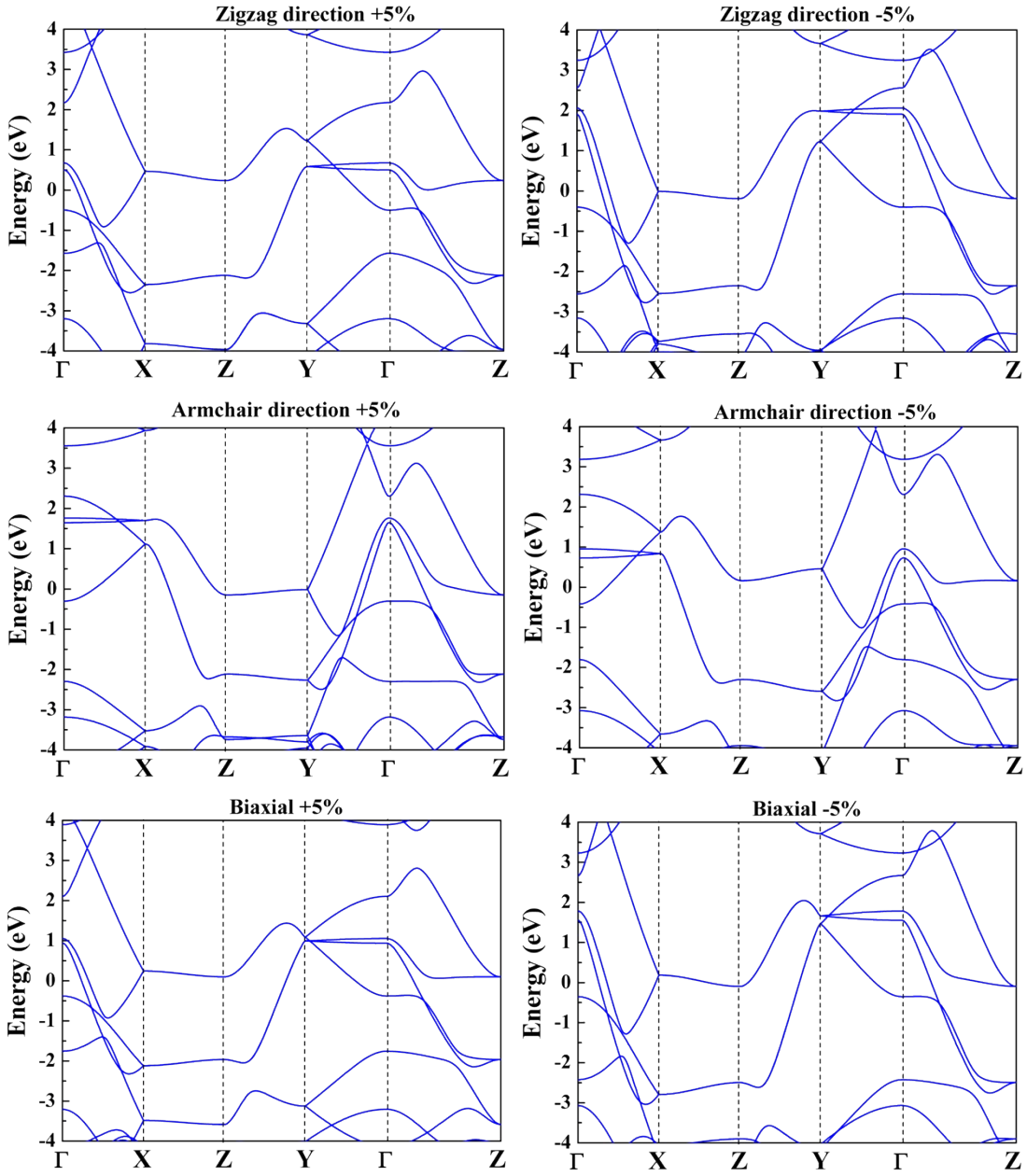

Figure S4. Adsorption structures of sixteen Li atoms on a popgraphene sheet after optimization with considering vdW corrections.

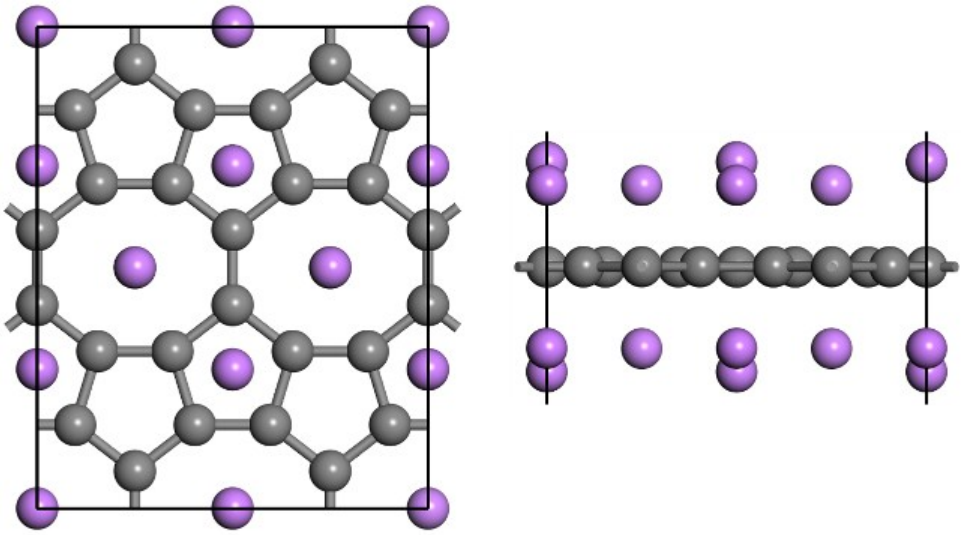

Figure S5. The fluctuations of total potential energy for $Li_4C_6$ during AIMD simulations at 300 K. Insets are top view (left) and side view (right) of snapshots of the equilibrium structure of $Li_4C_6$.

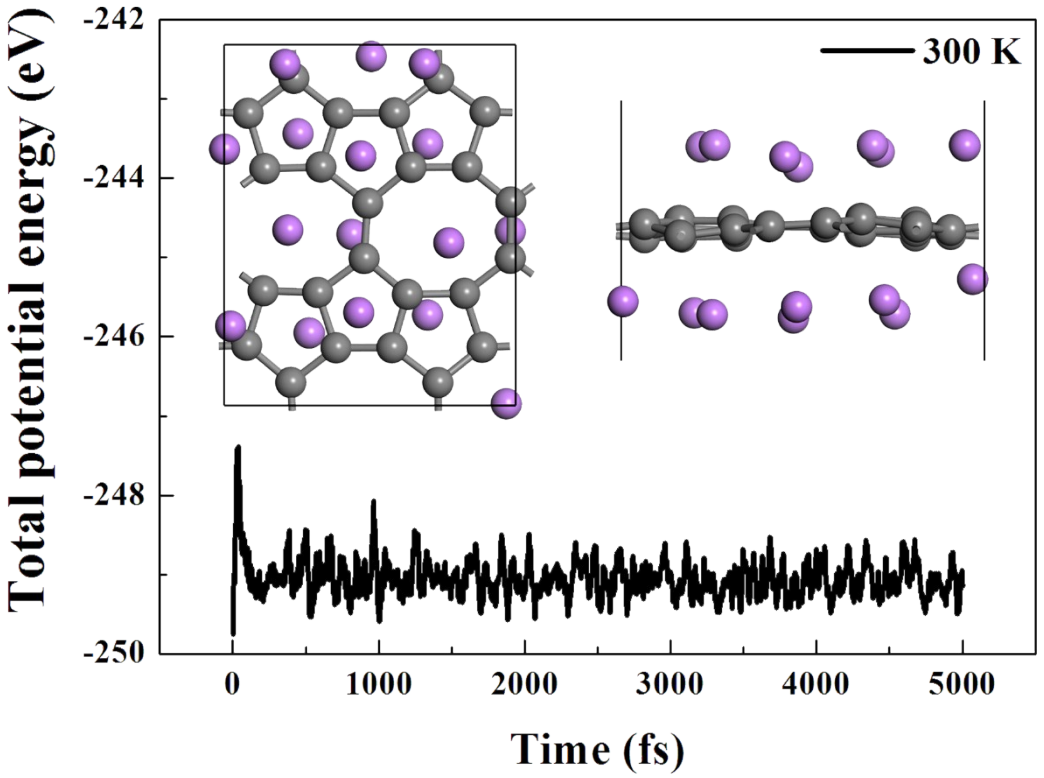

Figure S6. The corresponding diffusion energy profiles of Li diffusion on a popgraphene sheet without considering vdW corrections.