Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

Holey penta-hexagonal graphene: a promising anode material for Li-ion batteries

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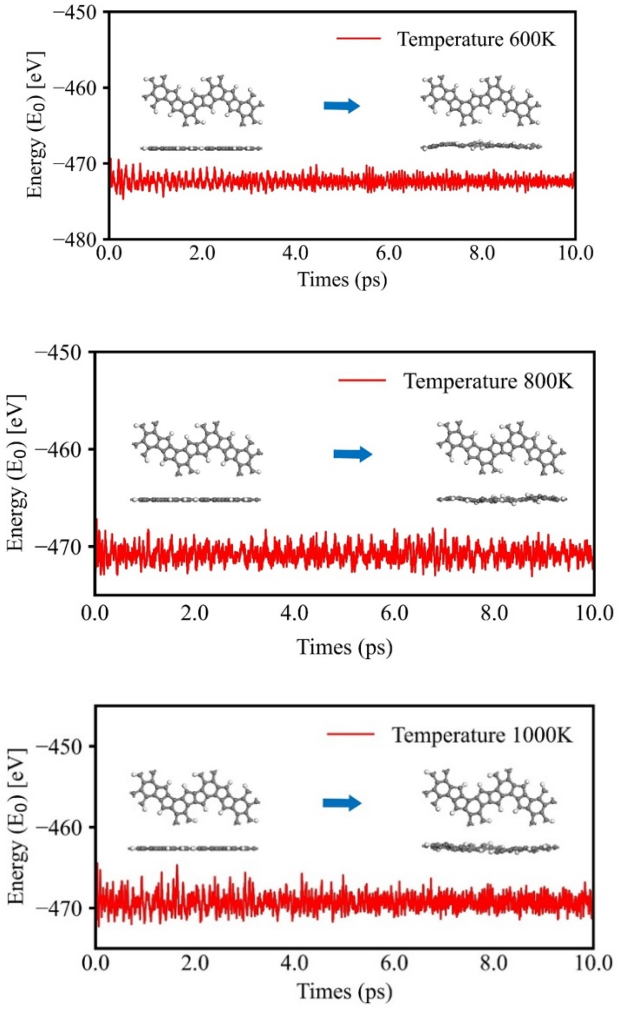

Figure S1. Initial and final structures of HPhG, accompanied by the energy evolution diagram, following a 10 ps AIMD simulation at 600 K, 800K, and 1000 K, respectively. The carbon and hydrogen atoms are denoted by grey and white, respectively.

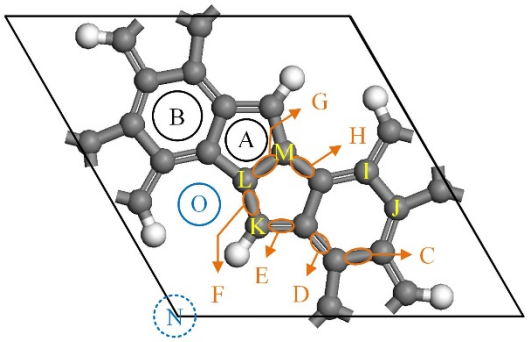

Figure S2. The possible Li adsorption sites in a unit cell of the holey penta-hexagonal graphene. The carbon and hydrogen atoms are denoted by grey and white, respectively.

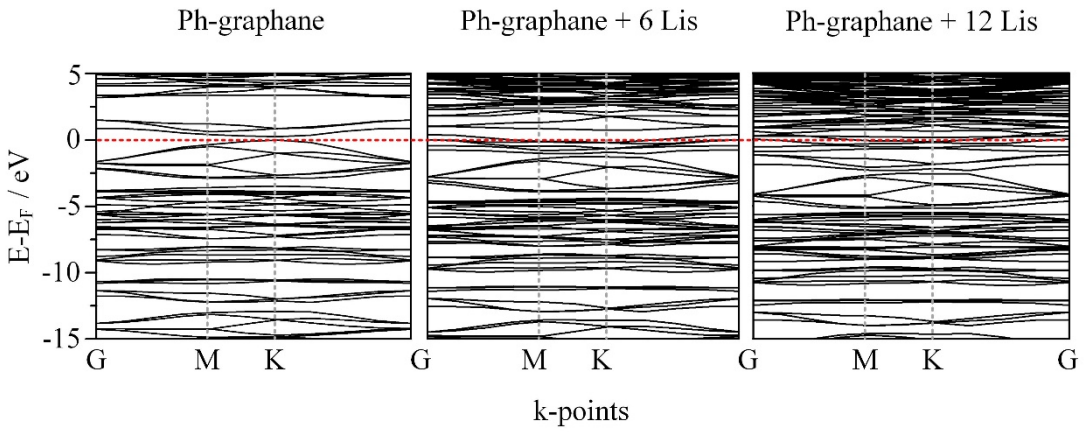

Figure S3. Band structures of holey penta-hexagonal graphene (HPhG) without and with adsorbed Li atoms (by PBE functional).

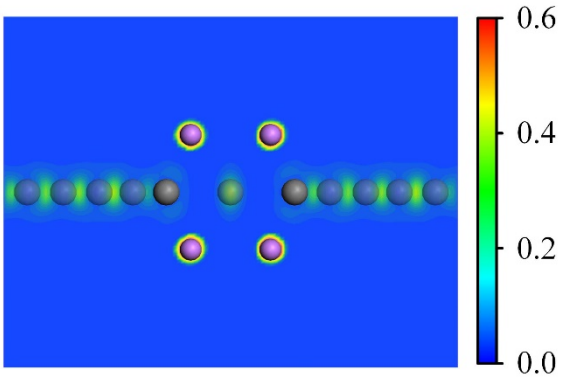

Figure S4. Electron location function (ELF) of holey penta-hexagonal graphene (HPhG) with 12 adsorbed Li atoms. The carbon, hydrogen and Lithium atoms are denoted by grey, white, and purple, respectively.