Supporting Information for

Topological semimetal porous carbon as a high-performance anode for Li-ion battery

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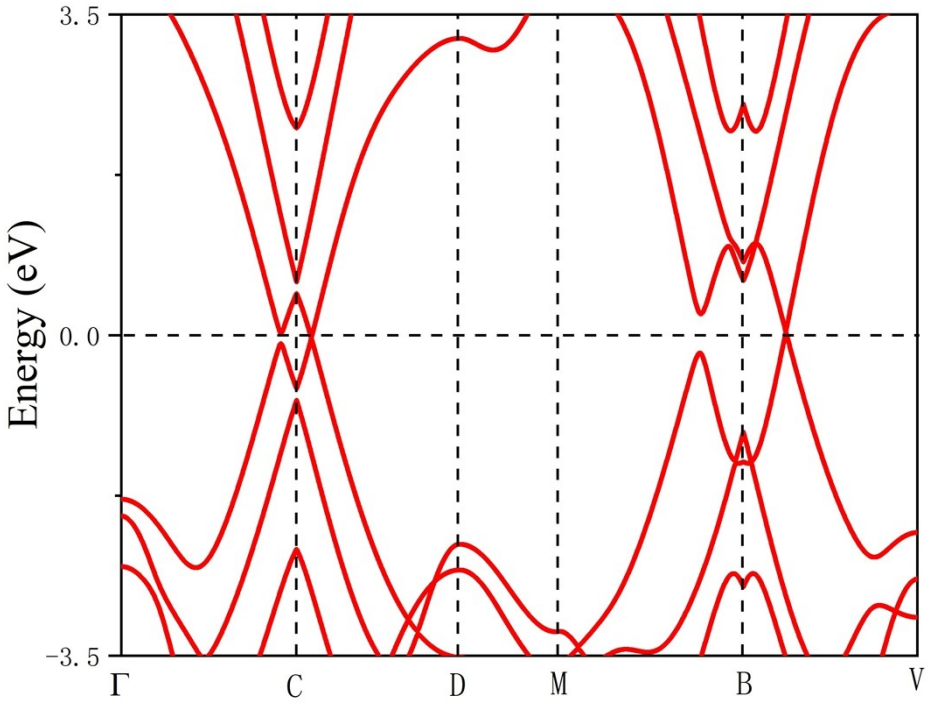

Figure S1: Calculated energy band structures along the high-symmetry points.

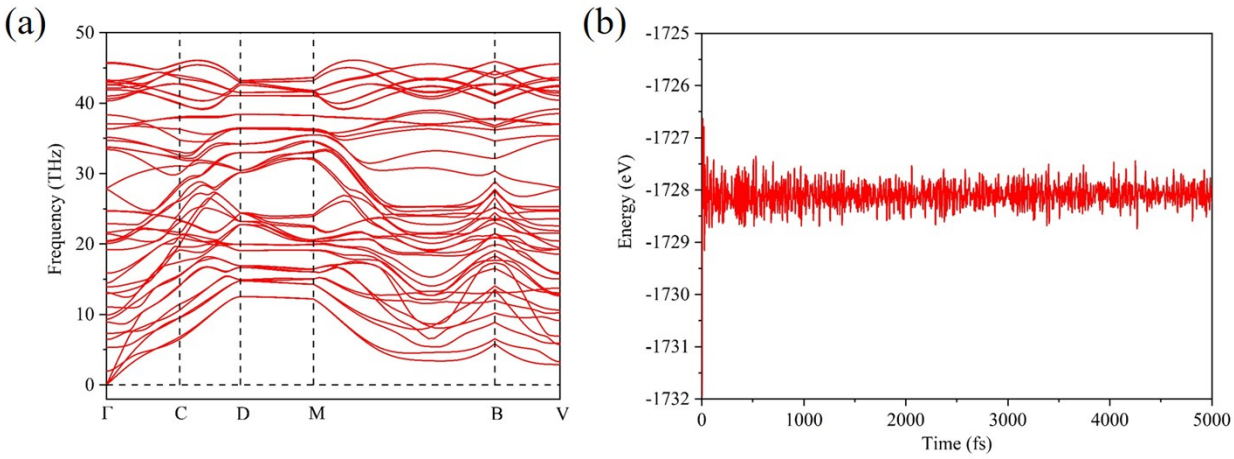

Figure S2: (a) Phonon spectra and (b) energy fluctuation during AIMD simulation at 300 K.

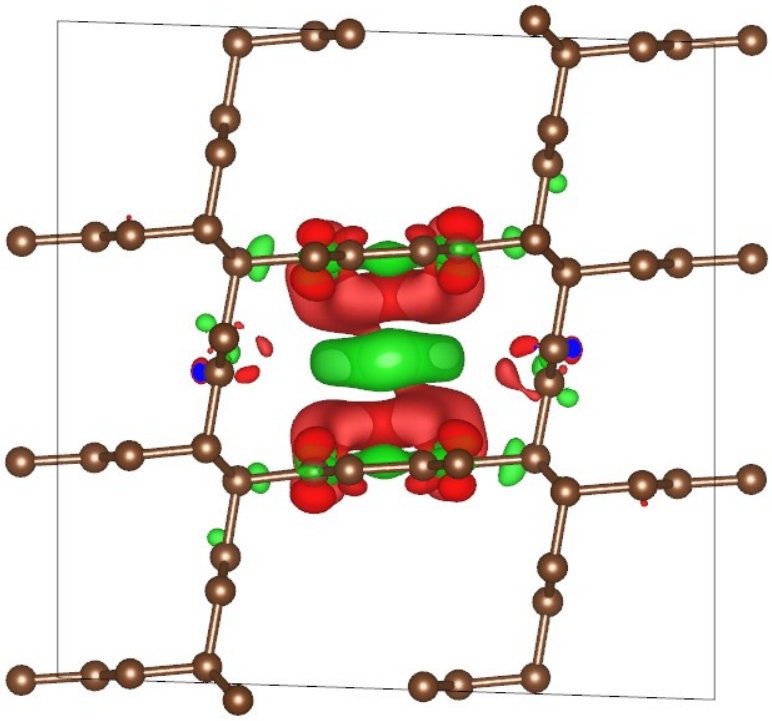

Figure S3: Charge density difference between the Li atom and the adsorbed system with an isosurface value of 0.004 e/Bohr^3. The red and blue are for charge gain and loss, respectively.

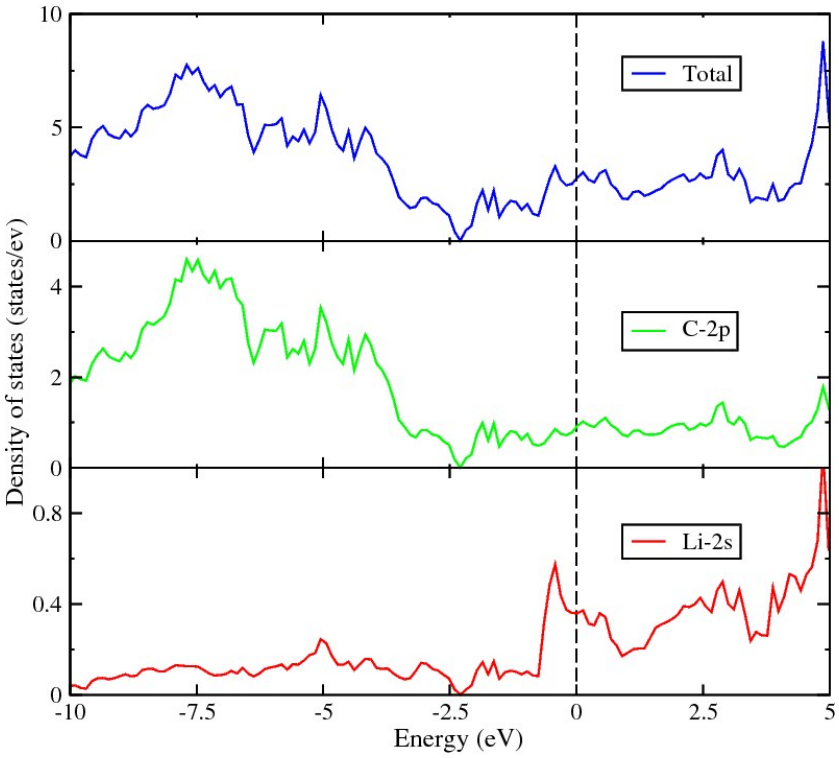

Figure S4: Total DOS and PDOS of the fully Li-intercalated m-C_{16}

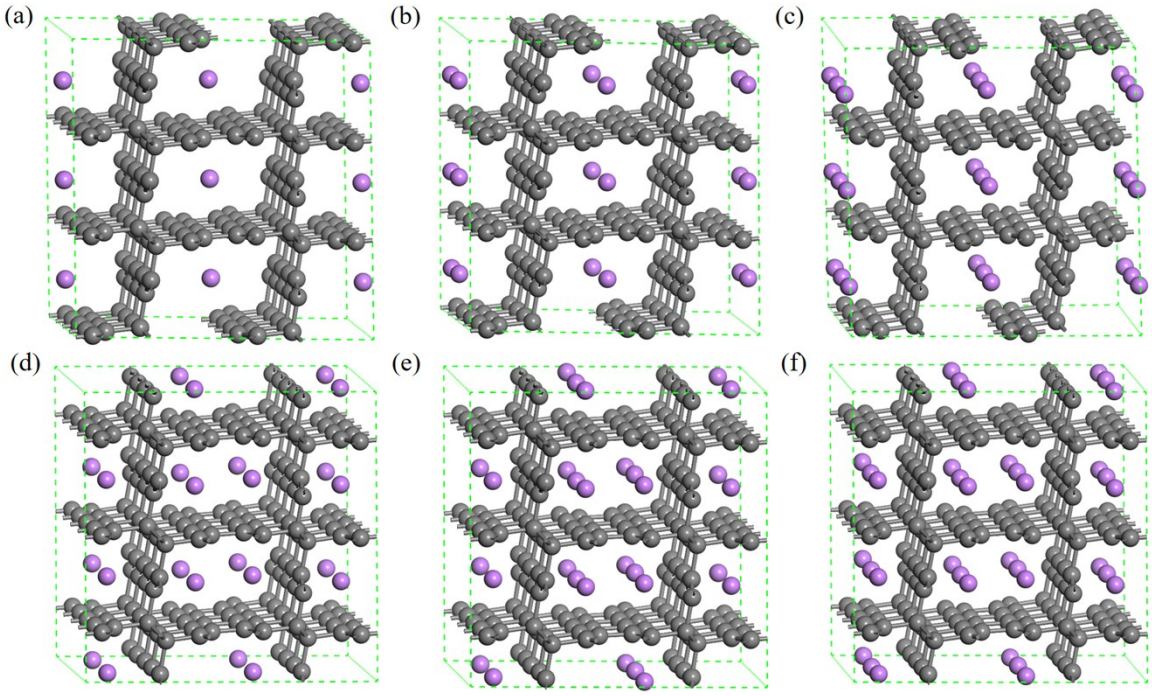

Figure S5: Side views of the six stable intermediate phases for the Li concentrations of (a) 0.125, (b) 0.25, (c) 0.375, (d) 0.5, (e) 0.625 and (f) 0.75.

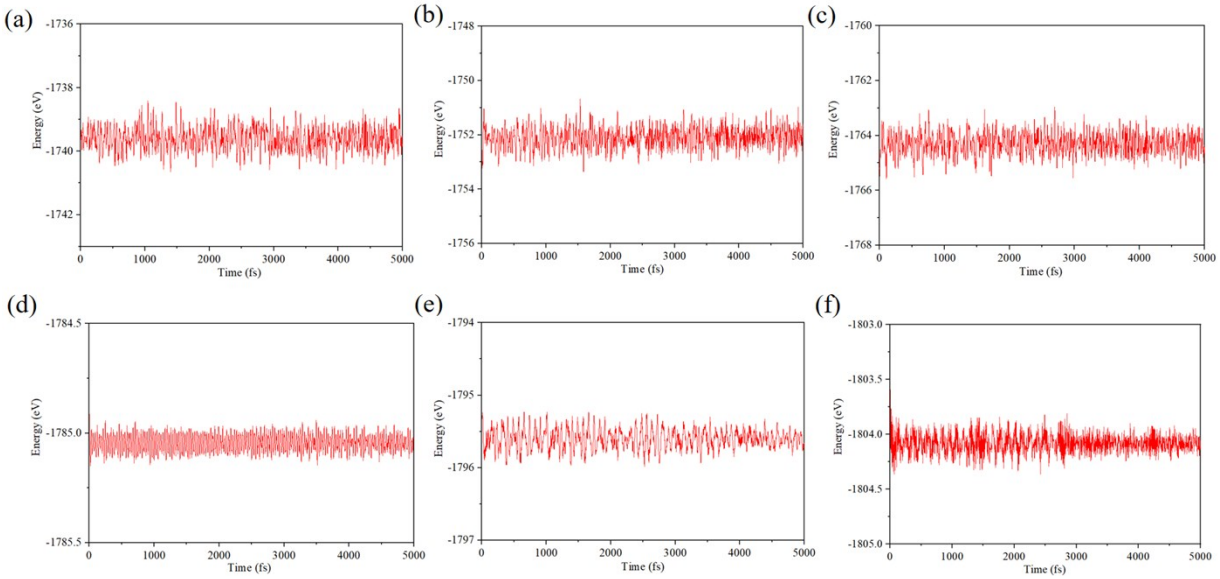

Figure S6: Energy fluctuation during AIMD simulation at 300 K of the six stable intermediate phases for the Li concentrations of (a) 0.125, (b) 0.25, (c) 0.375, (d) 0.5, (e) 0.625 and (f) 0.75.