Supporting Information

Acepentalene Membrane Sheet: A Metallic Two-Dimensional Carbon Allotrope with High Carrier Mobility for Lithium Ion Battery Anode

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Figure S1 The calculated phonon spectrum (a), the evolution of the potential energy versus time during the first-principles molecular dynamics simulation carried out at 1000 K (b), the stress-strain relationships for the uniaxial and equi-biaxial strains (c), and the corresponding energy surface versus the arbitrary in-plane strains (d). These results support high dynamic, thermal, and mechanical stabilities of the \( h \)-PAMS porous sheet. In (b), the insets are the configuration obtained at the end of the simulation (the left) and the after then optimized one at 0 K (the right). The depiction of the colored balls is the same as that in Figure 1.
Figure S2 The 2D carbon allotrope after the structural transition of $h$-PAMS obtained by loading $\varepsilon_d$ strain beyond 32%. The depiction of the colored balls is the same as that in Figure 1.
**Figure S3** The stacking configurations of the neighboring $h$-PAMS layers with the relative energies as referred to the ground state. The interlayer space is also provided below each configuration.
Figure S4 The adsorption of an excess Li on the Li$_3$C$_{10}$ in which the pre-adsorbed Li ions form the kagome configuration. The grey, blue, and red balls are for the carbon atoms, the pre-adsorbed Li ions, and the excess Li. The ground state adsorption is that the excess Li sits upon the pre-adsorbed Li ions developing three Li-Li bonds to show the tendency for surface clustering.
Figure S5 The Li intercalated $h$-PAMS bulk with only two neighboring $h$-PAMS layers are shown for illustration. The yellow and grey balls are for the carbon atoms in the lower and upper $h$-PAMS layers. The rhombic ring is the in-plane unit. The blue and red balls are the Li ions adsorbed upon the lower and upper $h$-PAMS layers, respectively. The pink balls mean that there are two Li ions adsorbed vertically along a line with one on the lower layer and the other one on the upper layer.
Figure S6 (a) The (0001) surface of Li$_3$C$_{10}$ bulk. (b) The adsorption of excess Li upon the trigonal Li layer. (c) The adsorption on the kagome lattice of Li layer. (d) The intercalation of the excess Li at the subsurface. The grey, blue, and red balls are for the carbon atoms, the Li ions of the Li$_3$C$_{10}$ bulk, and the excessively introduced Li atoms being obviously lifted up showing tendency for surface clustering. The newly introduced Li into the subsurface are hold at the same plane of the pre-adsorbed Li layer in (d), which are also accounted by the blue balls. Only the atoms in the vicinity of the adsorptions of the excess Li ions are highlighted while the others are only schematically illustrated by the skeleton using the grey line and blue plus symbols. The relative energies per unit cell containing only one excess Li adsorption are also provided in (c) and (d), as referred to the ground state in (b).