

Supplementary Information

A theoretical study for the performance evaluation of two-dimensional Carbon Kagome Lattice as an anode material for lithium-ion batteries

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AIMD simulation

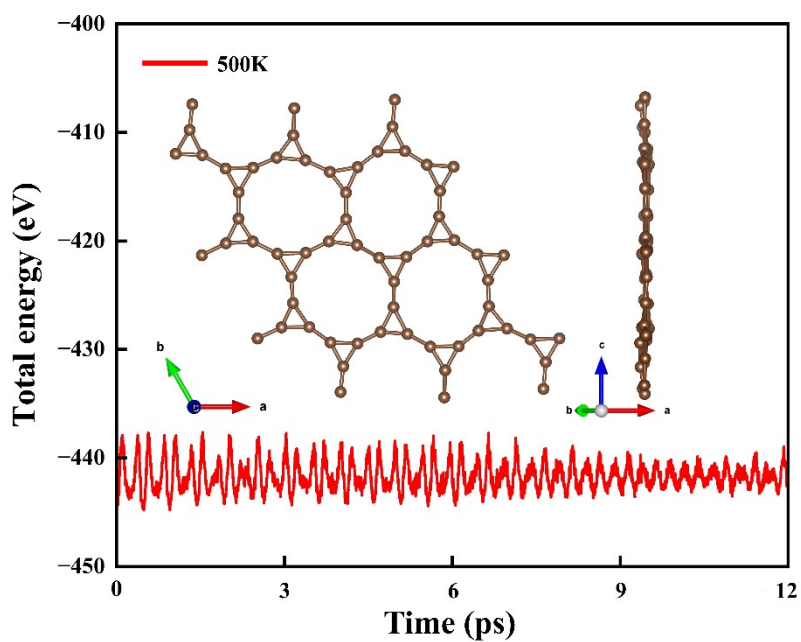


Fig. S1 Evolution of the total energy and final snapshot of CKL during an AIMD simulation at 500 K for 12 ps.

Projected crystal orbital Hamilton population (pCOHP)

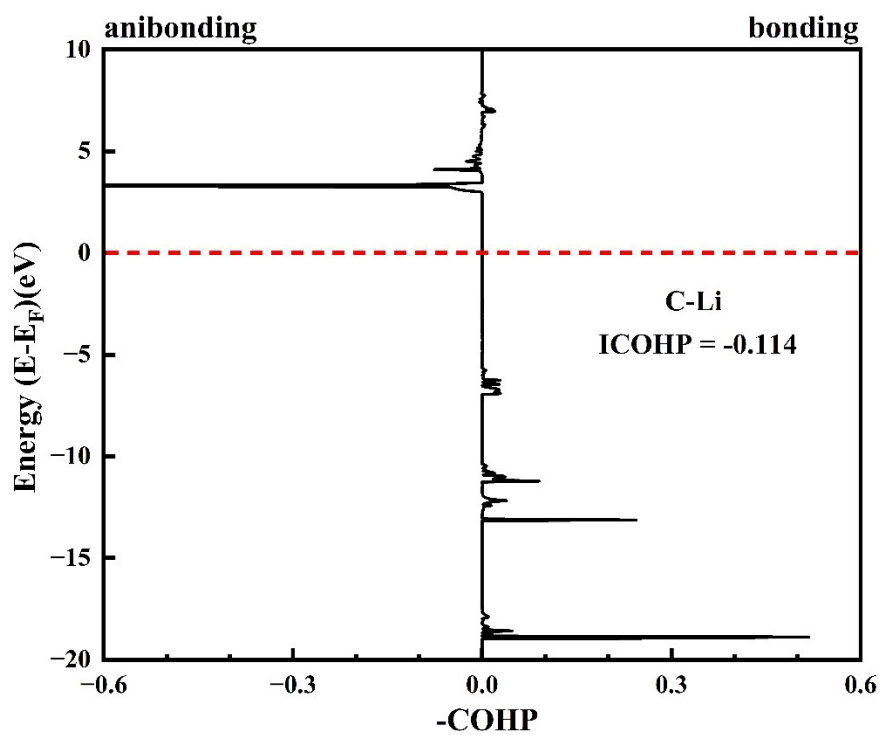


Fig. S2 -pCOHP curves of Li-C interactions at H1 site.