Identification of Crystal Structure and Lithium-Ion Storage Mechanism of Fluorinated-Contorted Hexabenzocoronene

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Organic electrochemical capacitor materials have attracted attention, because conductive polymer-based materials exhibit high conductivity and a high reversible redox reaction on the surface of electrodes. However, due to the poor stability in the aprotic electrolyte, organic electrode materials need to find alternatives. Herein, we used fluorinated cHBC (F-cHBC) to achieve the small-molecule-based organic capacitive energy storage cells, which can charge and discharge fast with high specific capacity. To identify the polymorph of F-cHBC crystal, a simulated annealing Monte Carlo simulation was performed. The in-silico polymorph screening revealed that the experimental X-ray diffraction (XRD) pattern of polymorph phase of F-cHBC closed matched the XRD pattern of the P21/c crystal phase. In addition, the lithiation process of P21/c crystal phase of F-cHBC was examined by DFT calculation with Monte Carlo simulation. We demonstrated that this high capacitive behavior of F-cHBC was mainly caused by the fluorine atoms at the end of each aromatic ring.