Theoretical Study on Lithium- and Sodium-Ion Storage of Fluorinated-Contorted Hexabenzocoronene

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As the demand for various types of energy storage devices increases, organic rechargeable batteries using organic materials as electrodes become a candidate of next generation energy storage systems due to the potential of design flexibility. Also, organic compounds have attracted much attention as electrochemical capacitor materials because they are sustainable, cost effective, and eco-friendly compared with conventional inorganic electrode. Thus, in this study, we used contorted hexabenzocoronene (cHBC) containing fluorine to achieve the small-molecule-based organic capacitive energy storage cells, which can charge and discharge fast with high specific capacity. We theoretically predicted the crystal phase of experimentally synthesized fluorinated cHBC (F-cHBC) with a Monte Carlo simulation method, by which the crystal structure of low lattice energy can be traced from the molecular structure. Lithiation and sodiation processes of F-cHBC were further examined by calculating formation energy of intercalated compounds and voltage profile in addition to identifying intercalation sites of lithium and sodium, through density functional theory calculation.