Computational Study on Organic Semiconductor C_{60}/cHBC Cocrystal for Highly Conductive Lithium Host Electrode

주세훈, 박주현, 박재현, 김윤정[1], 안석훈[1], 강석주, 곽상규†
울산과학기술원; [1]KIST
(skkwak@unist.ac.kr†)

Organic materials have attracted much attention as promising active materials for high-performance lithium-ion battery electrodes due to their low cost, feasibility as a Li^+ storage medium, high capability to transport electron, and the designing flexibility with electron-withdrawing/donating groups. Herein, we theoretically investigated an organic cocrystal of semiconducting fullerene (C_{60}) and contorted hexabenzocoronene (cHBC) as a conducting agent-free organic cocrystal anode material. The crystal structure of C_{60}/cHBC cocrystal was predicted through Monte Carlo (MC) simulation, which provided the information of the minimum-energy crystal structure from molecular structure. By performing density functional theory calculation in combination with the MC simulation, the Li storage mechanism of C_{60}/cHBC cocrystal was found through exploring the Li^+ adsorption sites and calculating the formation energy of Li-intercalated compounds. Finally, calculated voltage profile agreed well with the experimental result.