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Theoretical and Experimental Investigation of Binder-free Trimetallic Phosphate Nanosheets

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Abstract : Transition metal phosphides and phosphates are newly emerged electrode material candidates in energy storage devices. For the first time, we report uniformly distributed, interconnected, and well-aligned two-dimensional nanosheets made from trimetallic Zn-Co-Ga phosphate (ZCGP) electrode materials with preserved crystal phase. It is found that the ZCGP electrode material exhibits about 2.85 and 1.66 times higher specific capacity than mono- and bimetallic phosphate electrode materials at the same current density. The trimetallic ZCGP electrode exhibits superior conductivity, lower internal resistance (IR) drop, and high Coulombic efficiency compared to mono- and bimetallic phosphate. The charge storage mechanism is studied for mono- bi- and trimetallic electrode materials, which illustrate the diffusion-dominated battery-type behavior. By means of density functional theory (DFT) calculations, ZCGP shows superior metallic conductivity due to the modified exchange splitting originating from 3d-orbitals of Co atoms in the presence of Zn and Ga. Moreover, a hybrid supercapacitor (ZCGP//rGO) device is engineered, which delivered a high energy density (ED) of 40 W h kg^{-1} and a high-power density (PD) of 7,745 W kg^{-1}, lighting 5 different colors of light emitting diodes (LEDs). These outstanding results confirm the promising battery-type electrode materials for energy storage applications.

Keywords : trimetallic phosphate, nanosheets, DFT calculations, hybrid supercapacitor, binder-free, synergistic effect
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