Seminar

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Institute for Plasma Research

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Title: MOF-derived Transition Metal Compounds as Anode Materials for All-Solid-State Lithium-Ion Batteries

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Date: 29th November 2024 (Friday)

Time: 03.30 PM

Venue: Seminar Hall, IPR

Abstract

All-solid-state lithium-ion batteries (ASSLIBs) are viable alternatives to commercialized LIBs owing to their higher safety and better energy density. Herein, we have prepared Metal-Organic Framework (MOF)-derived transition metal phosphides & chalcogenides (TMPs & TMCs) as anode materials to achieve high capacity, long cyclability, and superior rate performance. For this, MOFs, including ZIF-67 cubes, ZIF-67 polyhedrons, and Fe-imidazole framework (Fe-MOF), were realized using facile chemical synthesis procedures, and they were then used as main precursors to create the sophisticated active materials by heat-treatment methods. $LiBH_4$ has been employed as a solid-state electrolyte in all the tests conducted in half-cell assemblies.

The investigations began with ZIF-67-based cobalt telluride particles surrounded with in-situ generated N-doped cubic carbon network (CoTe/NC) and polyhedron cobalt phosphide (Co_2P@NCF) nanocomposites. The Li-storage mechanism investigations of the prepared composite are revealed using ex-situ XRD and XPS techniques. The electrodes demonstrated conversion-cum-alloying mechanism during the first discharge scan, where CoTe and Co_2P formed Li_2Te and Li_3P upon lithiation, respectively. Meanwhile, the cobalt converts into the metallic Co and becomes redox inactive afterward. During the charging scan, the final lithiated products Li_2Te and Li_3P eventually convert into Te and LiP, respectively. Co_2P@NCF delivered a higher initial discharging capacity of 1705 mAh/g than its telluride counterparts which provided 1124.7 mAh/g at a current density of 100 μA. CoTe/NC also demonstrated excellent rate performance with ~ 92.3 % capacity retention after fast charging at various scan rates.

Motivated by the satisfactory performance of Co_2P@NCF, we continued exploring its cost-effective and environmentally friendly alternative, i.e., Fe-MOF-derived Fe_2P@NC nanocomposites. The composite anode delivered excellent initial discharging/charging capacities of 1214.8 mAh/g and 1367.01 mAh/g, respectively, at a current density of 100 μA. For Fe_2P, ex-situ XRD and XPS results also pointed out the formation of Li_3P and Fe in the first discharging cycle. Like Co_2P@NCF, in subsequent cycles, the reversible reaction $Li_3P \leftrightarrow$ LiP is found to be responsible for generating reversible capacities. The carefully evaluated electrochemical performance of MOF-based anodes with $LiBH_4$ electrolyte in ASSLIB indicates the profound possibilities of utilizing MOF-derived anode materials as futuristic anode materials for ASSLIB applications.