



Phase Stability and Transformation of Energy Storage Materials

SONG-MAO LIANG ^{1,8}, BIN OUYANG,² SHIH-KANG LIN,^{3,4,5,6}
and HANS J. SEIFERT⁷

1.—Computherm, LLC, Middleton, WI 53562, USA. 2.—Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA. 3.—Department of Materials Science and Engineering, National Cheng Kung University, Tainan 70101, Taiwan. 4.—Hierarchical Green-Energy Materials (Hi-GEM) Research Center, National Cheng Kung University, Tainan 70101, Taiwan. 5.—Program on Smart and Sustainable Manufacturing, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 70101, Taiwan. 6.—Core Facility Center, National Cheng Kung University, Tainan 70101, Taiwan. 7.—Institute for Applied Materials (IAM-AWP), Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

The demand for energy storage materials, such as used for high-performance batteries, supercapacitors, hydrogen storage, water splitting, photovoltaics, etc., is increasing exponentially. Phase stability is one of the major factors affecting the performance of the energy storage materials. In this issue on “Phase Stability and Transformation of Energy Storage Materials,” one review article and seven original research articles are compiled. The aim of this special topic is to introduce the development in energy storage materials from the aspect of phase stability and transformations.

Lithium batteries are widely used and extensively investigated energy storage devices. In the first article, “Issues, developments, and computation analyses of interfacial stability in all-solid-state Li batteries: A review,” Che-an Lin and Shih-kang Lin review the current status of the development of interfacial stability in all-solid-state Li batteries with a focus on the electrode/electrolyte contacts. Strategies for improving the contact stability are reviewed, such as employing protective layers and processes that can kinetically impede interfacial reactions. In addition, materials calculations for interface analyses and interface design in all-solid-

state batteries are highlighted, and the remaining challenges and outlook for further investigations are proposed.

In the research article “Ab initio interfacial chemical stability of argyrodite sulfide electrolytes and layered-structure cathodes in solid-state lithium batteries,” Yi-Tzu Wu and Ping-Chun Tsai use ab initio calculation to determine the interfacial stability of electrolytes $\text{Li}_6\text{PS}_5\text{A}$ (LPSA, A = Cl, Br, I) and cathodes Ni-rich $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ (LCO, NMC112, NMC333, NMC442, NMC811, and LNO) as a function of the state of charge (SoC). The results show that the interfacial chemical instability increases as the SoC increases. The interfaces between the LPSA electrolyte and NMC cathodes are predicted as thermodynamically unstable, and the chemical reactions are irreversible.

In the article “Spinel LiMn_2O_4 with remarkable electrochemical performances by synergistic enhancement of double-cation (Sm³⁺, Mo⁶⁺) doping for Li-ion batteries” Zhang et al. use a facile temperature solid-phase sintering method and successfully fabricate a Sm and Mo co-doped LiMn_2O_4 (LMO-Sm&Mo) cathode material for potential Li ion batteries application. The LMO-Sm&Mo shows better discharge capability (113.05 mAh g⁻¹) and prolonged cycling life (88.08%) than typical LMO (85.69 mAh g⁻¹ and 76.32%, respectively) after 200 cycles at 1 °C.

With the global trend of transitioning fossil energy to sustainable energy sources, generation of H₂ or energy storage from thermochemical water splitting mechanisms is intensively pursued by researchers. In the article “Investigation of Ca-

Song-Mao Liang, Bin Ouyang, Shih-kang Lin, and Hans J. Seifert are Guest Editors for the Alloy Phases Committee of TMS and organized the topic Phase Stability and Transformation of Energy Storage Materials in this issue.

(Received September 26, 2022; accepted September 28, 2022; published online October 17, 2022)

doped LaMnCoO_3 perovskite oxides for thermochemical water splitting,” Yiğiter and Pişkin investigated the phase stability of a series of Perovskite materials $\text{La}(\text{MnCo})\text{O}_3$ doped with Ca by XRD. Their results show that two Ca doped oxides, LCMC8282 and LCMC6482, possess high cycle stability and better H_2 generation ability than others.

For developing potential electrical energy storage materials, Kornphom et al. investigated the phase stability and energy storage performance of $0.722(\text{Bi}_{0.5}\text{Na}_{0.5}\text{TiO}_3)-0.228(\text{SrTiO}_3)-0.05(\text{AgNbO}_3)(\text{BNT-ST-AN})$ ceramics with various amounts of KF additions. In their article “High energy-storage performance under low electric fields and excellent temperature stability of KF-modified BNT–ST-AN relaxor ferroelectric ceramics” they report that BNT-ST-AN with KF addition at 0.15 mol% exhibits the best performance and shows great potential in pulse-power system applications.

SmCo_5 shows excellent magnetic properties, oxidation, and corrosion resistance, but the scarcity and high price of the Sm limit its applications in some special occasions. To find a cheaper rare earth replacement of Sm, in “Phase relations of the CeCo_5 - SmCo_5 pseudobinary system,” Xu et al. investigate the phase equilibria of a series of $(\text{Ce}_{1-x}\text{Sm}_x)\text{Co}_5$ alloys using scanning electron microscopy (SEM) equipped with energy-dispersive spectroscopy (EDS), x-ray diffraction (XRD), and differential thermal analysis (DTA). From the analytical results they constructed the SmCo_5 - CeCo_5 phase diagram

including the Curie temperature line, also based on the experimental results, together with previously reported data.

In another crucial Co-Cr-Zn alloy system, Wang et al. carried out extensive experimental work on 17 alloys which were heat treated at 450 °C for 2 months and 600 °C for 1 month to investigate the phase equilibria. As described in “Experimental investigation of the phase relations in the Co–Cr–Zn ternary system at 450 °C and 600 °C,” all the phases are identified by SEM with EDS and XRD. Then, the authors construct the isothermal sectional phase diagrams at 450 °C and 600 °C.

In “Novel hydrothermally synthesized strontium telluride nanoballs as: efficient electrocatalyst for oxygen evolution reaction” by Alfryyan et al., strontium telluride (SrTe/GC) nanoballs have been synthesized with hydrothermal synthesis. The as-synthesized material shows a low overpotential of 268 mV at 10 mA/cm^2 with a small Tafel slope of 25 mV/dec. The fabricated material exhibits excellent stability for 24 h with no decline in current density.

All titles and authors of the articles are published under the topic “Phase Stability and Transformation of Energy Storage Materials” in the December 2022 issue (vol. 74, no. 12) of JOM. The articles can be accessed fully via the journal’s page at: <http://link.springer.com/journal/11837/74/12/page/1>

Publisher’s Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.