Clarkson University
Department of Chemical and Biomolecular Engineering
SEMINAR

"Theoretical Investigation on the Sodiation Mechanism of Electrode Materials for Sodium-Ion Batteries"

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Sodium-ion batteries (SIBs) have emerged as an alternative to lithium-ion batteries (LIBs), particularly for large-scale energy storage, due to the abundant availability of Na resources and markedly low cost. In this work, promising anode and cathode candidates for SIBs are investigated to better understand the sodiation mechanisms by utilizing density functional theory (DFT) calculations. We first investigated the possibility of using P-doped and oxidized P-doped graphene as an anode material in SIBs. We reveal important fundamental properties of sodium adsorption on P- and oxidized P-doped graphene. Our results suggest that the Na capacity could reach 511 mAh/g with the P- and oxidized P-doped graphene anode which exceeds that of hard carbon anode in SIBs. Ionic and electronic transport properties were investigated to evaluate the rate capability and stable cyclability. Our findings indicate that P- and oxidized P- doping of graphene anodes could be a promising route toward increasing the overall performance of the SIBs for practical application.

We next investigated the sodiation mechanisms of selenium (Se), which is a promising cathode material for SIBs owing to its high electrical conductivity (~ 10-3 S/m) and facile sodiation kinetics. We first evaluate single Na incorporation in crystalline Se and formation of Na-Se alloys in terms of structural evolution, energetics, and mechanical properties at different levels of sodiation stage. Moreover, we also investigated the sodiation behavior of Se-graphene composites with a particular interest at the interface. Our calculations demonstrate a preferential Na adsorption at the interface and corresponding electrons transfer to both the graphene and Se atoms. Lastly, we will address the charge transport mechanism of the final discharge product Na2Se, which can limit the overall battery performance. Our results suggest that negatively charged Na vacancy is the main charge carrier due to its low formation energy and moderate energy barrier for diffusion. Our studies can provide fundamental understanding towards the efficient design of Se-based composites as promising cathode materials for SIBs.

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Sungwon Park is a Ph. D candidate in Chemical Engineering at Clarkson University. He received his bachelor's and master's degrees in Chemical Engineering at Inha University. His research focuses on computational modeling of advanced battery materials. He is particularly interested in sodiation mechanisms of electrode materials for sodium-ion batteries.