Graphitic SiC: A Promising Anode Material for Na-ion Battery with Extremely High Storage Capacity

Qin Liu[1], Bo Xiao[1], Yanchun Li[2], Jianbo Cheng[1], Zhenbo Liu[1], Xin Yang[1], Xiufeng Xu[1], and Qingzhong Li[1]

[1]Yantai University
[2]Jilin University

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Abstract

Bulk SiC phases with tetrahedral arrangements have been identified several decades ago, and have been widely studied due to their potential applications. Until recently, Yaghoubi et al.'s experimental results (Chem. Mater. 2018, 30, 7234) showed that the graphitic SiC with few SiC layers stacking is stable. In this work, we further explore the potential application of graphitic SiC as the Na-ion battery anode via the first-principle simulation. Our results reveal that the theoretical capacity of graphitic SiC reaches up to 1339.44 mAh/g, which is almost the highest among the already known Na-ion battery anodes. Together with the low diffusion barrier, moderate open circuit voltage and excellent electronic conductivity during the sodiation, we propose that the graphitic SiC is a promising material as Na-ion battery anode. More importantly, we find that the intercalation strength of Na ions into C-based multi-layer materials (or the corresponding theoretical capacity, the operation voltage) could be enhanced by increasing the amount of covalent components in Na-C bonds, which could be realized via doping by atom (such as Li, Be, B, Al, Si or P) with lower electronegativity than that of C atom.

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