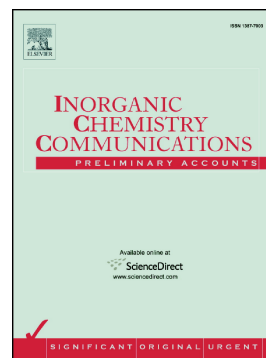


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Can the C_{32} and $B_{16}N_{16}$ nanocages be suitable anode with high performance for Li, Na and K ion batteries?

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Abstract

In this study, the potential of C_{32} and $B_{16}N_{16}$ as anode electrodes of Li-ion, Na-ion and K-ion batteries via density functional theory was investigated. The effects of C_{32} and $B_{16}N_{16}$ adoption with halogens on ability of metal-ion battery was examined. Obtained results show that $B_{16}N_{16}$ ($V_{cell} = 1.32$ V) as anode electrode in metal-ion batteries has higher potential than C_{32} ($V_{cell} = 1.15$ V). Calculated results illustrated that K-ion battery has higher cell voltage ca 0.15-0.30 V than Li-ion and Na-ion batteries. Results display that adoption with halogens increases the cell voltage of studied metal-ion batteries ca 1-1.5 V. Calculated results indicated that adopted metal-ion batteries with F have higher cell voltage ca 0.11-0.40 V than Cl and Br adopted metal-ion batteries. Finally it can be concluded that adopted F- $B_{15}N_{16}$ as anode electrode in K-ion battery has the highest performance and it can be proposed as novel metal-ion batteries with high performance.

Keywords: Battery, Nanocage, Adoption, Voltage, Anode and Halogen.

1 Introduction

Rechargeable batteries are a engaged nomination of stashing electricity in the appearance of chemical power and for convert the proceeding via converting that back to lightning [1-5]. A rechargeable battery is a kind of

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