Int. J. New. Chem., 2021, Vol. 8, Issue 4, pp. 425-441.

International Journal of New Chemistry
Published online January 2021 in http://www.ijnc.ir/.
Open Access

Print ISSN: 2645-7236

Online ISSN: 2383-188x

Article Type (Review Article or Original Research Article or Short Communication)

A density functional theory study on nanostructures including sumanene, corannulene and nanosheet as the anodes in Be−ion Batteries

Fatemeh Gharibzadeh[1], Esmail Vessally[2], Ladan Edjlali[1,*], Moosa Es'haghi[1], Robab Mohammadi [2]

[1] *Department of Chemistry, Tabriz Branch, Islamic Azad University, Tabriz, Iran*

[2] *Department of Chemistry, Payame Noor University, Tehran, Iran*

Received: 2021/03/17 *Accepted: 2021/06/19* *Published: 2021/09/15*

ABSTRACT

A theoretical study were performed to examine the interactions between the Be neutral atom and Be^{2+} ion and three sheet-Like nanoparticles such as sumanene (SM), corannulene (CN) and graphene, which are computed by M06−2X /6−31+G(d,p) method. The estimated values of adsorption energy (E_{ad}) are all negative in Be^{2+}– nanoparticles interaction. These results can be understood in terms of the electrostatic potentials of the negative sites on nanoparticles with which the positive regions on the Beryllium ion are interacting. In this article, the cell voltage (V) is the most important parameter for Be−ion batteries.It also determines the usability of a battery in an electrical system, and many battery parameters depend on voltage. Nevertheless, the Vcell for CN was obtained the highest value. The Vcell of Be−ion batteries are increased in the order: CN > SM > graphene > SM-i > CN-i. The mentioned nanoparticles as the anodes in BeiBs.

Keywords: nanoparticles, Sumanene, Corannulene, Nanosheet, Anodes in Be−ion Batteries, M06−2X/6−31+G(d,p) method, cell voltage

***Corresponding Author: Tel.: 09360221112**
OR 09352357794 E-mail: *l_edjlali@iaut.ac.ir*