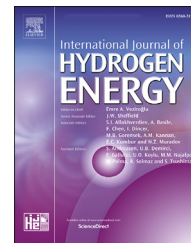


Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/ije

Perception of Mg adsorption on the BC₂N nanotube as a anode for rechargeable Mg ion batteries

Ghufran Sh. Jassim^a, Taleeb Zedan Taban^b, Mohanad Hatem Shadhar^c,
Mustafa M. Kadhim^{d,*}, Aiyah S. Noori^e,
Haider Abdulkareem Almashhadani^{f,g,h}, Ahmed Mahdi Rheima^{i,j},
Ali Mohamadi^k

^a Department of Chemistry, College of Science, University of Anbar, Anbar, Iraq

^b Laser and Optoelectronics Engineering Department, Kut University College, Kut, Wasit, 52001, Iraq

^c Department of Civil Engineering, Dijlah University College, Al-Masafi Street, Baghdad 00964, Iraq

^d Medical Laboratory Techniques Department, Al-Farahidi University, Iraq, Baghdad

^e Medical Physics Department, Al-Mustaqbal University College, Iraq

^f College of Medical Technology, Islamic University, Kufa Street, 54001 Najaf, Iraq

^g Dentistry Department, Al-Rasheed University College, Iraq

^h Medical Laboratory Techniques Department, Al-Turath University, Iraq

ⁱ Department of Chemistry, College of Science, Mustansiriyah University, Baghdad, Iraq

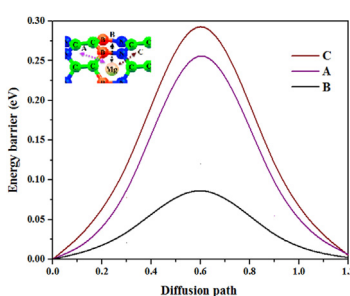
^j Medical Laboratory Techniques Department, Al-Turath University College, Iraq, Baghdad

^k College of Science, Islamic Azad University, Iran

HIGHLIGHTS

- DFT was performed for understanding the anodic properties of BC₂NNTs for MIBs.
- Mg preferably adsorbs on nearly B atom with E_{ad} −40.38 kcal/mol.
- The E_b have low values (0.07 eV), indicating that the MIBs in the BC₂NNTs.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 19 March 2022

Received in revised form

17 June 2022

Accepted 21 June 2022

Available online 13 August 2022

ABSTRACT

Owing to their cost-effectiveness and the natural abundance of magnesium, magnesium-ion batteries (MIBs) were introduced as encouraging alternatives to Lithium-ion batteries. Following the successful synthesis of carbon nano-tube, its B and N doped derivatives which were doped with B and N enjoyed the attention of researchers as novel anode materials (AM) for MIBs. Here, we investigated a BC₂N nano-tube (BC₂NNT) as an encouraging AM for MIBs. To have a deeper understanding of the electrochemical properties, cycling stability, specific capacity (SC) and the adsorption behavior of this nano-tube, first-

* Corresponding author.

E-mail address: Mustafa_kut88@yahoo.com (M.M. Kadhim).

<https://doi.org/10.1016/j.ijhydene.2022.06.203>

0360-3199/© 2022 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.