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Adsorption properties of graphene towards the ephedrine – a frequently used molecule in sport

Stevan Armaković^{1,*}, Sanja J. Armaković², Bogdan T. Tomić³,
Renjith Raveendran Pillai⁴, C. Yohannan Panicker⁵

¹ University of Novi Sad, Faculty of Sciences, Department of Physics, Trg D. Obradovića 4, 21000 Novi Sad, Serbia

² University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Trg D. Obradovića 3, 21000 Novi Sad, Serbia

³ Educons University, Faculty of Sport and Tourism – TIMS, Radnička 30a, 21000 Novi Sad, Serbia

⁴ Department of Physics, T.K.M. College of Arts and Science, Karicode, Kollam, Kerala, India

⁵ Department of Physics, Fatima Mata National College, Kollam, Kerala, India

* Corresponding author: Stevan Armaković, stevan.armacovic@df.uns.ac.rs

Abstract:

Adsorption properties of graphene nanosheet (GNS) towards the ephedrine (EPH) molecule, which belongs to a group of the most frequently used active components in sport supplements, have been investigated in details in this study. Different approaches within computational molecular modeling, including density functional theory (DFT), periodic DFT, time dependent DFT (TD-DFT) calculations and molecular dynamics (MD) simulations, have been applied. The study encompassed calculations of binding energies and detailed analysis of noncovalent interactions formed between GNS and EPH. Analysis of density of states and charge distribution was used in order to confirm that the physisorption mechanism is principally responsible for the EPH adsorption by GNS. MD simulations were used in order to determine which hydrogen atom of EPH had more important role in terms of interactivity with GNS. Spectroscopic properties were calculated and simulated in order to identify the most important changes occurring as a consequence of interactions between GNS and EPH. Obtained computational results indicate significant potential of GNS for practical applications for detection, delivery or removal of EPH.

Keywords: graphene; ephedrine; adsorption; DFT; TD-DFT; MD

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