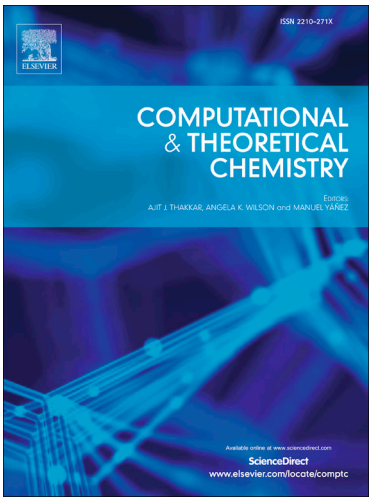

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PII: S2210-271X(17)30518-2
DOI: https://doi.org/10.1016/j.comptc.2017.12.009
Reference: COMPTC 2690

To appear in: *Computational & Theoretical Chemistry*

Received Date: 25 October 2017
Revised Date: 23 December 2017
Accepted Date: 24 December 2017

Please cite this article as: S. Armaković, S.J. Armaković, B.T. Tomić, R. Raveendran Pillai, C. Yohannan Panicker, Adsorption properties of graphene towards the ephedrine – a frequently used molecule in sport, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.12.009

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

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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