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Interaction of organic molecules and nanomaterials: Spectroscopic and theoretical insights into a weak-bound complex of hexagonal boron nitride and *trans*-stilbene

Ivan Halimski[1], Daniil Pashnev[1,2], Martynas Talaikis[1], Andrej Dementjev[1], Renata Karpicz[1], Jevgenij Chmeliov[1,3], Irmantas Kašalynas[1], Andžej Urbanovič[1,2], Yaraslau Padrez[1], Marijonas Tutkus[1,4,5], Patrizia Lamberti[6], Maksim Shundalau[6]

[1]*Center for Physical Sciences and Technology, Vilnius, Lithuania*
[2]*"Teravil" Ltd., Vilnius, Lithuania*
[3]*Institute of Chemical Physics, Faculty of Physics, Vilnius University, Vilnius, Lithuania*
[4]*Institute of Biotechnology, Life Sciences Center, Vilnius University, Vilnius, Lithuania*
[5]*"MB Platformina", Vilnius, Lithuania*
[6]*Department of Information and Electrical Engineering and Applied Mathematics, University of Salerno, Fisciano, Italy*
Email: mshundalau@unisa.it

2D and 0D hexagonal boron nitride (*h*BN) based materials are biocompatible and considered to be promising for applications in biomedicine for the bioimaging, targeted drug delivery, etc. For these purposes it seems important to provide quite strong adhesion of the molecule to the *h*BN surface on the one hand, and the possibility of its separation without disturbing the structure and loss of target properties on the other. Non-covalent interaction can ensure these conditions. Adsorbed molecules interact with surfaces due to relatively weak van der Waals interactions or electrostatic forces. *Trans*-stilbene (TST) is a non-polar and almost planar molecule, which suggests the possibility of pure non-covalent binding with the *h*BN surface, wherein covalent surface modification is practically excluded. Thus, the result of binding between TST and the *h*BN surface can be considered as a lower limit for this type of interaction and the TST can serve as a simple and almost ideal candidate to reveal the features of the formation of the complex between the *h*BN surface and organic molecules using spectroscopic and theoretical methods. Herein, we determine the main spectroscopic characteristics of a weak-bound complex of TST and *h*BN in different spectral ranges and techniques (THz, FTIR, Raman, CARS, and FL spectroscopy), find out the most appropriate spectroscopic methods to detect the complex formation. We also evaluate possibilities of different quantum chemical approximations (Gaussian and plane wave basis sets DFT calculations) for adequate modelling of structure and spectral characteristics of organic molecules adsorbed on the *h*BN surface.

The THz absorption spectra demonstrated the appearance of additional weak bands that can be assigned to the TST librations relative to the *h*BN surface. The TST + *h*BN Raman spectrum exhibits blue-shifted TST fingerprints lines. These trends were also predicted by DFT calculations. CARS microscopy technics was applied to check the complex structure. Weak complex formation could be also confirmed by the presence of a new 364 nm band in the FL spectrum and the slower FL decay kinetic. Based on the quantum chemistry calculations, we also concluded that dispersion forces are critical for the adsorption of the TST molecules on the *h*BN surface.

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