

**Список научных трудов
Петрушенко Игоря Константиновича
2016-2021 гг.**

Статьи:

1. Petrusenko I.K. Theoretical study on mechanical properties of polyethylene-SWCNT complexes // *Modern Physics Letters B*. – 2016. – V. 30. – N 3. – P. 1650012. DOI: 10.1142/S0217984916500123
2. Petrusenko K.B., Petrusenko I.K., Petrova O.V., Sobenina L.N., Ushakov I.A., Trofimov B.A. Environment-responsive 8-CF₃-BODIPY dyes with aniline groups at the 3 position: Synthesis, optical properties and RI-CC₂ calculations // *Asian Journal of Organic Chemistry*. – 2017. – V. 6. – P. 852-861. DOI: 10.1002/ajoc.201700117
3. Petrusenko I.K., Petrusenko K.B. Stone-Wales defects in graphene-like boron nitride-carbon heterostructures: Formation energies, structural properties, and reactivity // *Computational Materials Science*. – 2017. – V. 128. – P. 243-248. DOI: 10.1016/j.commatsci.2016.11.039
4. Petrusenko I.K., Petrusenko K.B. Physical adsorption of N-containing heterocycles on graphene-like boron nitride-carbon heterostructures: A DFT study // *Computational and Theoretical Chemistry*. – 2017. – V. 1117. – P. 162-168. DOI: 10.1016/j.comptc.2017.08.021
5. Petrusenko K.B., Petrusenko I.K., Petrova O.V., Sobenina L.N., Trofimov B.A. Novel environment-sensitive 8-CF₃-BODIPY dye with 4-(dimethylamino) phenyl group at the 3-position: Synthesis and optical properties // *Dyes and Pigments*. – 2017. – V. 136. – P. 488-495. DOI: 10.1016/j.dyepig.2016.09.009
6. Shipitsin N.V., Krivoshein A.I., Ivanov N.A., Petrusenko I.K., Rzhechitskii A.E. Thermally induced diffusion of F₂⁺ color centers in lithium fluoride crystals // *Journal of Luminescence*. – 2017. – V. 192. – P. 283-287. DOI: 10.1016/j.jlumin.2017.06.065
7. Petrusenko I.K. DFT Calculations of hydrogen adsorption inside single-walled carbon nanotubes // *Advances in Materials Science and Engineering*. – 2018. – V. 2018. – P. 9876015 (1-6). DOI: 10.1155/2018/9876015
8. Petrusenko I.K., Petrusenko K.B. DFT study of single-walled carbon hollows as media for hydrogen storage. // *Computational and Theoretical Chemistry*. – 2018. – V. 1140. – P. 80-85. DOI: 10.1016/j.comptc.2018.08.001
9. Petrusenko I.K., Petrusenko K.B. Hydrogen adsorption on graphene, hexagonal boron nitride, and graphene-like boron nitride-carbon heterostructures: A comparative theoretical study // *International Journal of Hydrogen Energy*. – 2018. – V. 43. – N 2. – P. 801-808. DOI: 10.1016/j.ijhydene.2017.11.088
10. Petrusenko I.K. Physical adsorption of N-containing heterocycles on hexagonal boron nitride: DFT-D₃ study // *Journal of Nano- and Electronic Physics*. – 2018. – V. 10. – N 2. – P. 02010 (1-6). DOI: 10.21272/jnep.10(2).02010
11. Petrusenko I.K., Petrusenko K.B. Effect of methyl substituents on the electronic transitions in simple *meso*-aniline-BODIPY based dyes: RI-CC₂ and TD-CAM-B₃LYP computational investigation // *Spectrochimica Acta – Part A: Molecular and Biomolecular Spectroscopy*. – 2018. – V. 190. – P. 239-245. DOI: 10.1016/j.saa.2017.09.025
12. Petrusenko I.K., Petrusenko K.B. Adsorption of diatomic molecules on graphene, h-BN and their BNC heterostructures: DFT study // *Diamond and Related Materials*. – 2019. – V. 100. – P. 107575. DOI: 10.1016/j.diamond.2019.107575
13. Petrusenko I.K. A DFT study of hydrogen adsorption on h-BN: Boron doping effects // *Journal of Nano- and Electronic Physics*. – 2019. – V. 11. – N 2. – P. 02024 (1-5). DOI: 10.21272/jnep.11(2).02024
14. Petrusenko I.K., Tsar'kova A.I., Tikhonov N.I., Petrusenko K.B. Valine adsorption on pristine and N-doped graphenes: DFT, AIM, and IGM study // *Material Research Express*. – 2019. – V. 6. – P. 125061. DOI:10.1088/2053-1591/ab5841

15. Petrushenko I.K., Petrushenko K.B. Optical properties of bilayer quantum dot models based on coronene and its BN analogues with a BODIPY dye: Theoretical TD-CAM-B₃LYP-D₃ investigation // *Spectrochimica Acta – Part A: Molecular and Biomolecular Spectroscopy*. – 2019. – V. 206. – P. 498-505. DOI: 10.1016/j.saa.2018.08.033
16. Petrushenko I.K., Petrushenko K.B. Hydrogen physisorption on nitrogen-doped graphene and graphene-like boron nitride-carbon heterostructures: a DFT study // *Surfaces and Interfaces*. – 2019. – N 17. – P. 100355. DOI: 10.1016/j.surfin.2019.100355
17. Petrushenko I.K., Petrushenko K.B. Physical adsorption of hydrogen molecules on single-walled carbon nanotubes and carbon-boron-nitrogen heteronanotubes: A comparative DFT study // *Vacuum*. – 2019. – V.167. – P. 280-286. DOI: 10.1016/j.vacuum.2019.06.021
18. Petrushenko I.K., Tikhonov N.I., Petrushenko K.B. Graphene-BN-organic nanoflake complexes: DFT, IGM and SAPT0 insights // *Diamond and Related Materials*. – 2020. – V. 107. – P. 107905. DOI: 10.1016/j.diamond.2020.107905
19. Petrushenko I.K., Tsar'kova A.I., Petrushenko K.B. Hydrogen adsorption on BN-embedded tetrabenzopentacene as a promising nanoflake for energy storage: Theoretical insights // *Diamond and Related Materials*. – 2020. – V. 108. – P. 107968. DOI:10.1016/j.diamond.2020.107968
20. Petrushenko I.K., Shipitsin N.V., Petrushenko K.B. Cation- π interactions of inorganic benzenes with Li, Na, and Mg cations: Theoretical insights // *Inorganic Chemistry Communications*. – 2020. – V. 118. – P. 108043. DOI: 10.1016/j.inoche.2020.108043
21. Petrushenko I.K., Petrushenko K.B. Absorption properties of a BODIPY-curved graphene nanoflake system: A theoretical investigation // *Spectrochimica Acta – Part A: Molecular and Biomolecular Spectroscopy*. – 2020. – V. 224. – P. 117465. DOI: 10.1016/j.saa.2019.117465
22. Petrushenko I.K., Petrushenko K.B. Absorption and fluorescence properties of non-symmetric benzo-, furo-, and thieno-fused structures at the *b* bonds in the BODIPY frame // *Spectrochimica Acta – Part A: Molecular and Biomolecular Spectroscopy*. – 2020. – V. 239. – P. 11847. DOI: 10.1016/j.saa.2020.118472
23. Petrushenko I.K., Tikhonov N.I., Petrushenko K.B. Hydrogen adsorption on pillar[6]arene: a computational study // *Physica E: Low-dimensional Systems and Nanostructures*. – 2021. – V. 130. – P. 114719 (1-7). DOI: 10.1016/j.physe.2021.114719
24. Petrushenko I.K., Petrushenko K.B. Evaluating mutual influences of cation- π interactions and H-bonding: cases of indole and BN-indole // *Polyhedron*. – 2021. – V. 200. – P. 115131 (1-7). DOI: 10.1016/j.poly.2021.115131
25. Petrushenko I.K., Petrushenko K.B. Theoretical predictions of the spectroscopic properties of BODIPY dyes: effects of the fused aromatic and heteroaromatic rings at the *b,g* bonds // *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*. – 2021. – V. 247. – P. 119125 (1-8). DOI: 10.1016/j.saa.2020.119125