# Accepted Manuscript


Optical properties of bilayer quantum dot models based on coronene and its BN analogues with a BODIPY dye: Theoretical TD-CAM-B3LYP-D3 investigation

I.K. Petrushenko, K.B. Petrushenko

| | |
|---|---|
| PII: | S1386-1425(18)30806-0 |
| DOI: | doi:10.1016/j.saa.2018.08.033 |
| Reference: | SAA 16408 |
| To appear in: | *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* |
| Received date: | 31 May 2018 |
| Revised date: | 7 August 2018 |
| Accepted date: | 19 August 2018 |

Please cite this article as: I.K. Petrushenko, K.B. Petrushenko , Optical properties of bilayer quantum dot models based on coronene and its BN analogues with a BODIPY dye: Theoretical TD-CAM-B3LYP-D3 investigation. Saa (2018), doi:10.1016/j.saa.2018.08.033

# Optical properties of bilayer quantum dot models based on coronene and its BN analogues with a BODIPY dye: Theoretical TD-CAM-B3LYP-D3 investigation

Petrushenko I.K.[a*] and Petrushenko K.B.[b]

[a]Irkutsk National Research State Technical University, 83 Lermontov st., Irkutsk 664074, Russia.

[b]AE Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, 1 Favorsky st., Irkutsk 664033, Russia.

*Corresponding author

## Abstract

Quantum dots (QD) belong to a class of materials considered technologically important for their tunable absorption and emission properties and a huge application potential in optoelectronic technologies. To date, only simplified monolayer models of QDs and their dimers have been considered when modeling their absorption and/or emission spectra and effects of edge functionalization.

Here, we analyze the optical properties of new type electron donor-acceptor bilayer quantum dot models based on coronene and its boron-nitride analogues (an electron donors) with a 4,4-difluoro-4-bora-3a,4a-diaza-s-indacene dye (**Bdp**, an electron acceptor) dye by using time-dependent density functional theory. To understand the nature of transition shifts in electronic spectra, we use BN models with strong modification of the HOMO and LUMO: **m-BNC** (middle hexagonal ring CC bonds are substituted by BN), **p-BNC** (all peripheral CC bonds are substituted by BN), and **f-BNC** (all C atoms are replaced by B and N in an alternate manner). Adiabatic ionization potentials of all coronenes were also calculated.

The obtained results show that significant interlayer charge transfer (CT) on excitation of bilayer QDs in $S_1$, $S_2$, and $S_3$ states from strong electron donors, coronene (6.93 eV) and **m-BNC** (6.52 eV), to **Bdp** will occur. As a result, one can observe only very weak absorption of CT-character in the low-energy spectrum region as well as strong fluorescence quenching of **Bdp**. On the contrary, for the weak electron donors, **p-BNC** (7.22 eV) and **f-BNC** (8.22 eV), strong **Bdp**-like absorption and fluorescence bands of local excitation character in the low-energy region are expected.

Correlation of optical properties of bilayer QDs with ionization potentials of coronene monolayers has been founded. The obtained results can be useful for future graphene-based optoelectronic applications.