3rd National Congress on Physical Sciences, 29 Sep. – 2 Oct. 2016, Sofia
Section: Physics of Condensed Matter, New Materials, Cryogenic Physics

Excitonic Spectra of Hexagonal 2D Compounds

I.J. Lalov, **I. Zhelyazkov**

Faculty of Physics, University of Sofia, BG-1164 Sofia

Abstract. In this paper, we consider the models and perform simulations of the excitonic spectra of two 2D structures of donor–acceptor (DA) compounds, notably: (i) graphene-like DA model in which the nodes of a hexagonal lattice are occupied by D molecules while the A molecules occupy the other non-equivalent positions (e.g., Lalov & Zhelyazkov, Bulg. J. Phys. **42** (2015) 172–199). That structure has been realized in a 2D crystal of hexagonal Boron Nitride; (ii) the model of Mxenes (transition metal carbides). We explore the case DA2 of A molecules in the nodes of a hexagonal 2D lattice whereas the D molecule are located on the nodes of a trigonal lattice dual to the hexagonal one (their positions coincide with the centers of the hexagons).

Two types of excitons have been studied in both models: (a) Frenkel excitons that stem from the electronic excitation of D or A molecules, and (b) charge transfer excitons (CTEs) of the ionized pairs of closest DA molecules (3 branches in model (i) and 6 branches in model (ii)). We analyzed the coupling of both types of excitons for dipole-active combination with transition electric dipole moment perpendicular to the layer or parallel on the lattice. The linear absorption spectra in excitonic and vibronic regimes have been calculated and simulated.