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Excitons in two-dimensional boron nitride[1]

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This work presents the theoretical study of the exciton problem in the two-dimensional hexagonal boron nitride (hBN). The dispersions of the conduction and valence bands are described by using the tight-binding approximation (TBA) with the model parameters extracted from the *ab initio* dispersions. The self-consistent equation for the interband electron-hole propagators is shown to have four contributions which are first order in the Coulomb interaction: Hartree, Fock, ladder and RPA contribution. In the long wavelength limit only the ladder contribution is relevant resulting in the standard hydrogen atom like Schrödinger equation. This approximation overestimates the exciton binding energies by one order of magnitude.

Therefore, it is necessary to include high-order contributions by replacing the bare Coulomb interaction in ladder diagrams with the screened interaction [1]. This leads to the self-consistent exciton energy eigenvalue problem with dynamical screening. This model predicts the dependence of the exciton energy on the angular quantum number. The higher value of angular momentum has lover energy for the same principal quantum number. The results are compared to the optical absorption experiments [2]. It turns out that the bare band gap must be larger then the gap obtained by the ab initio calculations.

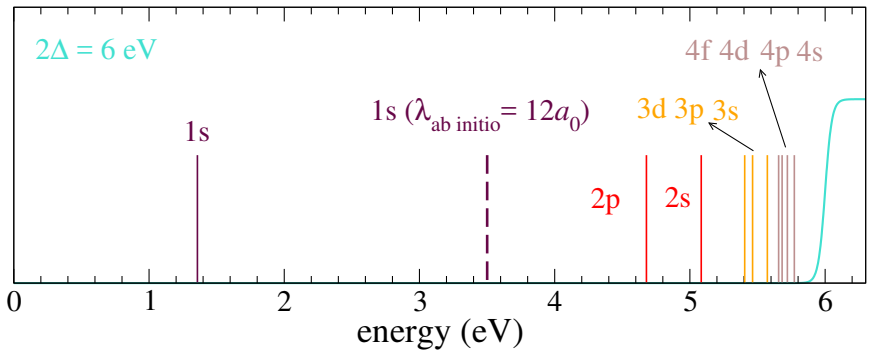

Figure 1: The excitonic spectrum of hBN containing first ten levels (solid lines) calculated using the TBA model. The dashed maroon line represents the ground state exciton calculated by using the *ab initio* static polarizability. The threshold energy for the single particle excitations is represented by the turquoise line.

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[2] L. Maseur et. al., Phys. Status Solidi **5**, 214 (2011).

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