Direct/indirect band gap and exciton dispersion: monolayer and bulk hexagonal boron nitride

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Among layered materials, hexagonal boron nitride (hBN) has remarkable optical properties owing to its wide band gap and strongly localized excitons. Theoretical calculations [1,2,3] agree in predicting a transition from direct to indirect band gap from the monolayer to the bulk, analogously to what observed in transition metal dichalcogenides. However, this prediction contrasts with the observation of high emission rates [4,5,6].

In this work, we address this issue from the theoretical point of view. Rather than analysing the single-particle band structure, we focus our analysis directly on the exciton dispersion in hBN. Many body perturbation theory (GW approximation and Bethe-Salpeter equation) has been employed to investigate the excitonic properties of the hBN monolayer and its variations passing to the bulk phase, with the intent of disclosing the connections between the dimensionality of the material, the single-particle band structure and the exciton dispersion.

Our results agree very closely with recent experimental and theoretical data [6,7,8], they cast a new light onto the excitonic properties at q≠0 and provide a possible explanation of the high luminescence efficiency.

References

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Figures

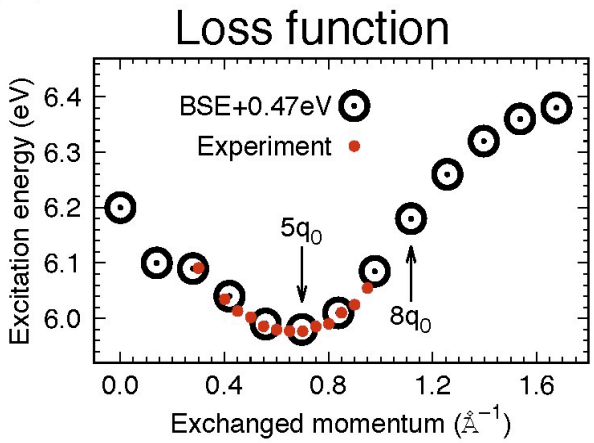

Figure 1: Computed dispersion of the first exciton of the loss function and comparison with experiments [6,7].