Modeling excitons in bulk and single-layer hBN

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Since the synthesization of graphene monolayers, the domain of 2D materials has experienced a continuously increasing interest owing to the many peculiarities exhibited by 2D materials. Among them, remarkable optical properties are of great interest. To gain a deep understanding of the dielectric response at the atomic scale is an essential step toward an efficient functionalization of these materials.

Hexagonal Boron Nitride (hBN) can be synthesized in the form of 2D films sharing the same honeycomb structure as graphene but presenting semiconducting properties. These features make hBN a promising candidate for technological applications (alone, doped or within C-based heterostructures). Nevertheless, the fundamental mechanisms of light-absorption in hBN are still not completely understood, not even in the bulk.

In this work I present a fine analysis of theoretical simulations of the excitonic effects on bulk and single-layer hBN.
To account for excitons in 2D hBN, we developed a model based on a tight-binding approach and we compared its predictions with the ab-initio solution of the Bethe-Salpeter equation [1,2,3].
As for the bulk system, we characterised the principal excitonic peaks by comparing BSE results with independent-particle transitions. Moreover the ab-initio spectra have been useful to validate our novel experimental setup, intended for optical spectroscopy measurements on ultra-thin films [4].

References

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Figures

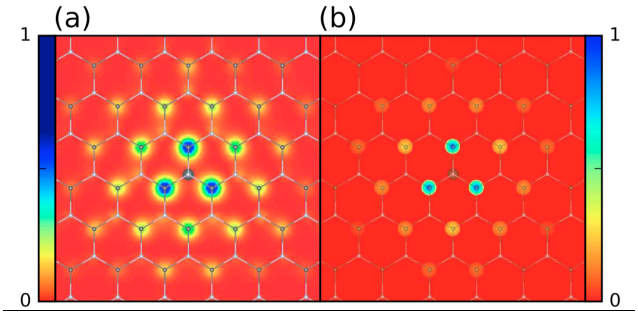

Figure 1: (a) ab-initio and (b) tight-binding model of the first exciton in single-layer hBN [1].

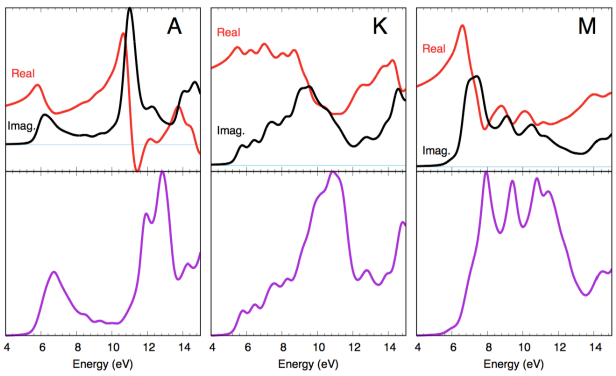

Figure 2: (top panels) Dielectric function and (bottom panels) loss function of bulk hBN at different momentum transfer.