Excitons in disordered Boron Nitride

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Hexagonal Boron Nitride (hBN) is a two-dimensional material well-known for its strong excitonic effects. Recently, defects in hBN have attracted considerable attention for application in optoelectronics, such as single-photon emitters. Concurrently, *amorphous* Boron Nitride (aBN) has been identified as an ultralow dielectric constant material with potential for next generation interconnects [1]. There is thus at present a need for methods to compute the excitonic properties of large disordered systems, and investigate the interplay between disorder, electron-hole Coulomb interaction and dielectric screening. Using BN as a prototypical system, we start from a tight-binding (TB) description of its electronic structure and perturbatively map the Bethe-Salpeter equation onto an effective TB Hamiltonian [2]. We are then able to extract relevant properties of large systems at a low computational cost by means of real-space linear scaling techniques (KPM, recursion…) [3,4]. As proof of concept, we discuss optical absorption in hBN in the presence of Anderson disorder a well as a toy model of structurally disordered BN based on aBN geometries obtained by molecular dynamics [5].

References

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