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Ab initio calculations of optical properties of complex 2D van der Waals Heterostructures

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Abstract

I will describe a number of recently developed computational methods to predict the optical properties of van der Waals heterostructures containing hundreds of atoms in a unit cell. To obtain the single-particle band structure, we employ a layer-projected scissors (LAPS) operator that incorporates short and long-range electron self-energy effects and ensures a proper description of the band alignment at the interface [1]. I will show that the LAPS method yields an accuracy comparable to the many-body GW approximation, but at the cost of a standard density functional theory (DFT) calculation. To compute the optical excitations, we solve the Bethe-Salpeter Equation (BSE) using a minimal basis for the electron-hole states. The screened Coulomb interaction is calculated using a mixed quantum-classical electrostatic model. By using a hierarchical basis comprising dielectric eigenstates of the individual monolayers, we can converge the BSE calculations using only a handful of basis functions. Combining these methods, we perform a high-throughput screening to identify vdW heterobilayers with interesting excitonic properties. The calculated data is made available in the open heterostructure database HetDB [2,3], which is integrated with the C2DB monolayer database [4].

[1] Dario A. Leon *et al*., arXiv:2505.17292 (2025)

[2] https://hetdb.fysik.dtu.dk

[3] M. O. Sauer *et al.* arXiv:2504.05754

[4] https://c2db.fysik.dtu.dk