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Recent Progress in GW-based Methods for Excited-State Calculations of Reduced Dimensional Systems[1]

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Ab initio calculations of excited-state phenomena within the GW and GW-Bethe-Salpeter equation (GW-BSE) approaches allow one to accurately study the electronic and optical properties of various materials, including systems with reduced dimensionality. However, several challenges arise when dealing with complicated nanostructures where the electronic screening is strongly spatially and directionally dependent. In this talk, we discuss some recent developments to address these issues. First, we turn to the slow convergence of quasiparticle energies and exciton binding energies with respect to k-point sampling. This is very effectively dealt with using a new hybrid sampling scheme, which results in savings of several orders of magnitude in computation time. A new *ab initio* method is also developed to incorporate substrate screening into GW and GW-BSE calculations. These two methods have been applied to mono- and few-layer $MoSe_2$, and yielded strong environmental dependent behaviors in good agreement with experiment. Other issues that arise in confined systems and materials with reduced dimensionality, such as the effect of the Tamm-Dancoff approximation to GW-BSE, and the calculation of non-radiative exciton lifetime, are also addressed. These developments have been efficiently implemented and successfully applied to real systems in an *ab initio* framework using the BerkeleyGW package.

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