GW-BSE Calculation of the Optical Response of Spin Polarized Materials and Nanostructures

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Many-body perturbation theory (MBPT), such as the GW approximation [1,2] and Bethe-Salpeter equation (BSE)[3], has been shown to be reliable for obtaining quasiparticle band structures and optical responses of solids. However, the spin-dependent optical properties of materials have not been well studied in the context of MBPT until now. In this talk, we will give an overview of developing the GW-BSE method with the spin degree of freedom included.

As examples, we present first-principles calculations of the optical properties of zigzag-edged graphene nanoribbons (ZGNRs) and NiO employing the GW-BSE approach with the spin interaction included. For ZGNRs, in addition to the large binding energy of electron-hole pairs, the edge-state excitons are charge-transfer and spin-transfer excitons, which provides a means to modify the magnetization optically [4,5]. For NiO, the quasiparticle band structure and optical responses are studied by the above spin-polarized GW-BSE method. The calculated density of states is in a good agreement with experimental measurements. Significant excitonic effects are found in the calculated optical spectrum of NiO, which also improves the agreement with experimental measurements [6].

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