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GW/Bethe-Salpeter Calculations for Solids for Core and Valence Spectra

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The introduction of self-energy corrections to density- functional calculations has greatly improved the one-electron properties of materials. GW calculations are a prime example of this. Excitation spectra, meanwhile, often probe the excited states of materials that involve the excitation of at least one electron across the Fermi level, producing an electron-hole pair. This can be the case for optical absorption and inelastic scattering of x-rays and electrons. Because of interactions in the excited state between the electron and hole, it is preferable to solve the coupled two-particle equation of motion for the electron-hole pair. Bethe-Salpeter-equation (BSE) calculations are a prime example of this. In addition to solving the equation of motion for an interacting electron and hole moving in a static solid, one can try to include lifetime- damping and other effects in the absorption spectrum. In this talk, I would like to present a framework that allows treatment of excitation spectra in a wide variety of materials, ranging from traditional semiconductors and insulators to fairly complicated minerals. This will also facilitate consideration of uniaxial birefringence, spatial-dispersion-induced birefringence, multiplet effects, and electric-quadrupole transitions in x-ray spectra.