Many-electron Correlations in Multi-particle Excitations and Nonlinear Optical Processes in Materials

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Excited-state phenomena in a material typically give rise to its defining attributes and determine its usefulness. These phenomena are particularly important in processes of energy conversion, transport and storage. However, *ab initio* methods for them - especially for correlated multiple-particle (3- or 4-particle) excitations, nonlinear optical processes, and electron dynamics including relevant electron-electron interactions - have been under-explored and hence limiting their studies for real materials. In this talk, we report recent progress on the *ab initio* theory and computation of such excited-state phenomena based on the interacting Green's functions approach to many-body perturbation theory. We present: 1) our new formalism and computational method for 3- and 4-particle correlated excitations with applications to trions and biexcitons in reduced-dimensional materials; and 2) our development of a time-dependent GW approach for time-dependent processes and nonlinear optics, which has led to the discovery of giant exciton effects in shift currents in two-dimensional semiconducting materials.