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Pushing the limits of the GW-BSE methodology for complex materials, molecules and nano-systems.

The GW-BSE approach, a many-body Green's function approach to spectroscopic properties, as currently practiced has been restricted to systems or unit cells with about 100 atoms because of computational limits. The difficulty is further exasperated for molecular systems by the need to include thousands of empty states in the continuum for the construction of the polarizability and the need to include hundreds of off-diagonal elements of the self-energy operator to accurately compute the unoccupied quasiparticle states. We show that, through a combination of methodological and algorithmic developments, the standard GW-BSE approach can now be applied to systems with 500-1000 atoms (or equivalently 100 AU x 100 AU x 100 AU unit cells). The advance is achieved through a combination of innovations: 1) improving the starting point of the GW-BSE approach through the use of hybrid functionals and/or self-consistent COHSEX quasiparticle states; 2) minimizing the expense of computing empty-state wavefunctions through various physical modeling such as static remainder computations and mixed basis representation; and 3) employing new algorithms/load strategies that give nearly linear parallel scaling to thousands (and beyond) of CPUs on current and future high performance supercomputers. It is shown that nowhere does the code scale worse than N^3. We will present concrete examples of real material applications, such as excitons in the optical response of the (21,21) carbon nanotubes and large molecules, to illustrate the capabilities of the method.