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Time-dependent density-functional theory for electronic excitations in materials[1]

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There is currently an intense effort underway to study the optical properties of bulk and nanostructured materials using time-dependent density-functional theory (TDDFT). This talk will discuss challenges and recent advances of TDDFT in this area, and present some new applications to excitonic effects in bulk insulators and to collective charge- and spin-density excitations in doped quantum wells. A TDDFT version of the semiconductor Bloch equations is presented, which describes ultrafast electron dynamics, including excitonic effects, in insulators and semiconductors. From this, an excitonic Wannier equation is derived featuring a nonlocal effective electron-hole interaction determined by long-range exchange-correlation effects. Excitonic binding energies are calculated for several direct-gap insulators. The spin Coulomb drag (SCD), which constitutes an intrinsic source of dissipation for spin currents in metals and semiconductors, originates as a dynamical exchange-correlation effect in time-dependent current-DFT. We develop a linear-response description of collective spin-density excitations in quantum wells including SCD as well as Rashba and Dresselhaus spin-orbit coupling, and show that spin plasmon line widths in quantum wells allow a purely optical, quantitative measurement of the SCD effect.

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