Real-space Calculations of Optical Constants from UV to X-rays*

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There has been substantial progress in recent years both in calculations and in the interpretation of x-ray absorption spectra (XAS). For deep core x-ray absorption, an independent-electron approximation with final state potentials including a core-hole is often adequate [1]. However, corrections to the independent particle approximation due to local fields are often important, especially for soft-x-ray energies. These local fields arise from the screening of the external x-ray field and the coupling to the core-hole, and require a treatment that goes beyond the independent-electron approximation. We have developed an efficient approach for treating these effects in solids and molecules based on a combination of the Bethe-Salpeter equation (BSE) and time-dependent density functional theory (TDDFT) [2]. This combined approach has been implemented within the real space Green's function method, and makes possible efficient calculations of optical constants from the UV to x-ray energies in aperiodic systems. These constants include the dielectric function, absorption and energy loss spectra, as well as related quantities like x-ray scattering factors. The extension to finite momentum transfer, e.g., non-resonant inelastic x-ray scattering is also discussed [3].

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