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Combined BSE/TDDFT approach for x-ray absorption calculations[1] A.L. ANKUDINOV, Y. TAKIMOTO, J.J. REHR, University of Washington — Many-body effects such as local fields and the core-hole interaction can be significant in x-ray absorption spectra, even several hundred eV above an absorption edge. The treatment of these effects requires theories that go beyond the independent particle approximation such as the Bethe-Salpeter equation (BSE) or time-dependent density functional theory (TDDFT). However, neither of these approaches is fully satisfactory; the BSE is usually restricted to low energies while the TDDFT ignores non-locality. Here we present a combined TDDFT/BSE approach which is applicable over a wide spectral range. This approach is implemented within a real-space multiple-scattering formalism, with core-hole interaction and the local screening fields calculated within linear response. The approach is illustrated for a several materials and compared with experiment, including the Mg K-edge of MgO, the Ni L-edges, and W M-edges.

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