

Ab initio results for the valence-hole effects in RIXS from cBN

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Soft x-ray emission spectra for resonant inelastic x-ray scattering (RIXS) in cubic boron nitride are computed. In RIXS, a core electron is excited by an x-ray into the conduction bands, and as a result, fluorescence is radiated from the recombination of the core hole and a valence electron. For the first time, we realistically take into account both the core hole effects in the intermediate states and the valence-hole "exciton" effects in the final states. Our ab initio results show strong enhancement because of core hole effects in the intermediate states and more importantly valence hole effects in the final states if the incident photon energy is below the B K edge, while very little enhancement observed if the incident energy is above the edge. This highlights electron correlation effects and helps clarify remaining discrepancies between experiment and theory.