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Ab initio calculation of core-valence-valence Auger spectra in closed shell systems. GIAN PAOLO BRIVIO, GUIDO FRATESI, MARIO ITALO TRIONI, Universita' di Milano-Bicocca, SIMONA UGENTI, ENRICO PERFETTO, MICHELE CINI, Universita' di Roma Tor-Vergata, MILANO-BICOCCA COLLABORATION, ROMA TOR-VERGATA COLLABORATION —
We propose an ab initio method to evaluate the core-valence-valence Auger spectrum of systems with filled valence bands. The method is based on the Cini-Sawatzky theory, and aims at estimating the parameters by first-principles calculations in the framework of DFT. Photoemission energies and the interaction energy for the two holes in the final state are evaluated by performing DFT simulations for the system with varied population of electronic levels. Transition matrix elements are taken from atomic results. The approach takes into account the non spherical density of states of the emitting atom, spin-orbit interaction in core and valence, and non quadratic terms in the total energy expansion with respect to fractional occupation numbers. It is tested on two benchmark systems, Zn and Cu metals, leading in both cases to $L23M45M45$ Auger peaks within 2 eV from the experimental ones. Especially problematic is the evaluation of the hole-hole interaction for systems with broad valence bands: our method underestimates its value in Cu, while we obtain excellent results for this quantity in Zn.

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