

Abstract Submitted
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Density Matrix Approach for Valence Band Optical Properties¹

M.P. PRANGE², J.J. REHR, University of Washington — We present an extension of the *ab initio* real-space multiple-scattering (RSMS) theory currently used for core-level spectra (e.g. EELS, XAS and NRIXS) to calculations of the valence band optical response. The method is based on RSMS calculations of the occupied and unoccupied density matrices and transition matrix elements between the two resulting in an efficient way to calculate various optical constants in aperiodic materials. In contrast to bandstructure or basis-set methods, the calculation can be applied to a large class of materials including both insulators and metals up to the nanoscale. By combining the method with the RSMS approach for core level response, we obtain an approach applicable for spectra from the far IR to x-rays. Results are compared with experiment and with other theoretical techniques. Possible extensions are also discussed.

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