

Abstract Submitted
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Optical Matrix elements in empirical tight-binding with overlap

TITUS SANDU, Chemical and Materials Engineering Department, Arizona State University, Tempe, AZ — Calculations of optical and electronic properties of materials are mostly carried out making two assumptions: an orthogonal, atom-like basis and a diagonal coordinate operator in this basis. Thus the intra-atomic matrix elements of coordinate operator are neglected. We show that including the overlap between the orbitals, intra-atomic contributions between different orbitals on the same atom are considered.

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