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Perturbative second-order optical susceptibility of bulk materials: a symmetry-enforced return to non-orthogonal localized basis sets

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The second-order optical susceptibility of semiconductors $\chi_{ijk}^{(2)}$ finds application in metrology, spectroscopy, telecommunications, material characterization, and quantum information. Pioneering calculations of $\chi_{ijk}^{(2)}$ utilized non-orthogonal Gaussian orbitals centered at atoms. That formulation transitioned into plane-wave-based algorithms as time went by. As of late, nevertheless, multiple tools for calculating optical susceptibilities have recast the problem using Wannier (i.e. localized) orbitals, making a comeback onto frameworks based on localized basis sets. Here, we present an approach for calculating $\chi_{ijk}^{(2)}$ reliant on numerical pseudo-atomic orbitals (PAOs) within perturbation theory in the velocity gauge. Its salient feature is a calculation of 'Slater-Koster-like' two-center integrals of the momentum operator in between PAOs identified by symmetry. The approach was successfully tested on paradigmatic cubic silicon carbide (3C-SiC) and gallium arsenide, for which linear responses are contributed as well.

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