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Computational Strategies for Deciding NLO Properties

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Abstract: *Non-linear optical (NLO) materials have garnered significant attention in recent years due to their potential applications in photonics, optoelectronics, and quantum computing. Accurate estimation of NLO properties, such as second- and third-order nonlinear susceptibilities, is crucial for designing and optimizing these materials. Computational strategies, including density functional theory (DFT), time-dependent DFT (TDDFT), and post-Hartree-Fock methods, have emerged as powerful tools for estimating NLO properties. These abstract reviews recent advances in computational strategies for estimating NLO properties, highlighting their strengths, limitations, and applications. We also discuss perspectives on future developments, including the integration of machine learning algorithms and the exploration of new materials with enhanced NLO properties.*

Keywords: DFT, TDDFT, NLO. Gauss view

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