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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

I. INTRODUCTION

In recent years, there has been substantial demand for organic molecules with high nonlinear optical properties than inorganic materials in current use for optical devices. The main cause is that the better performance of the organic materials than the best inorganic materials in order of magnitude. As a consequence, there is a demand for theoretical characterization of nonlinear organic materials. Hence interests in searching and designing new organic materials with the desired linear and nonlinear optical properties.

The objective of this article is to calculate the linear and nonlinear optical properties of organic materials from a first principle. The brief history of the first principle started in In 1926 E. Schrödinger published the paper on wave mechanics and presented the Schrödinger equation for the wave function Ψ of electrons [1].

In 1998 Nobel Prize in chemistry was awarded to John A. Pople for his development of computational methods in quantum chemical techniques embodies in the Gaussian electronic structure codes and to Walter Kohn for his development of the density-functional theory (DFT)[2].Both quoted In their Nobel lectures, a famous remark made by Dirac in 1929 for the successful of the ultimate theory of many electrons by wave-mechanics:

"The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known," Unluckily, his amusing statement continues. "And, the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved." As an attempt to solve the complex equation from the first principle ab initio Schrödinger produced not only wave-mechanics of electrons electronic structure as an attempt to solve the complex equation. The first working programmable digital computer used in 1938 when Konrad Zuse built the first electro-mechanical binary programmable computer called Z1 with all facilities.

Although Dirac could perhaps not imagine today's exponential progress in digital computing power, his remark that the full treatment of the Schrödinger -Dirac equation is so complicated to solve exactly, except for very small molecules is still correct. About all of these strategies begin from compelling one-electron models in which electrons move freely (Hartree Fock technique) [3] encountering just an average potential because of the impact of other electrons, core nuclei, and external fields. These one-electron wave functions are named atomic orbitals, and since molecules are consist of atoms, an extremely viable procedure has been to grow the molecular orbitals as far as atom-centered atomic orbitals. Unquestionably, this linear combination of atomic orbitals (LCAO) strategy [4] has been accountable for many

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of accomplishments of the initial fifty years of quantum chemistry. The ab initio methods for potential electronic structure can be categorized into two classes. The first category includes wave function-based methods, namely post-Hartree Fock schemes in the the framework of Configuration Interaction or Coupled Cluster schemes which can be used for molecules containing up to a few atoms and are likely to give accurate results. The second category includes density-based methods (DFT) which cover systems between a few tens up to a few hundreds of atoms. It is regularly of far-reaching appropriateness and sensibly precise in numerous cases.

II. PRINCIPAL METHODS FOR THE STUDY OF ELECTRONIC STRUCTURE

There are three primary ways to deal with molecular properties -

i) ab initio methods [5] ii) Semi empirical method [6] and iii)molecular mechanics method [7,8] (Error! Reference source not found.)Schrödinger equation is the fundamental equation as a basic of all Quantum chemical models. It considers molecule as pool of nuclei and electrons, without any considering chemical bonds. The elucidation of the Schrödinger equation is in terms of the motions of electrons, which in turn leads directly to molecular structure and energy among other observables, as well as to information about bonding. However, the Schrödinger equation cannot actually be solved for any electron system (except hydrogen atom), and approximations need to be made. Quantum models vary in the idea of these approximations, and traverse a wide range, both as far as their capacity, consistency, and their cost. The first approximation made is separatel the electronic motion for the nuclear motion.

This was a wonderful approximation since the electrons are significantly lighter than the nuclei and instantly modify their movement to an adjustment in the position of the nuclei. We would then be able to write an expression for the electronic energy of the electrons in the fixed electrostatic field of the nuclei:

Ee(R) = Ekin + Eelec-nuc + Eelec-elec(1)

The energy Ee (R) is written as a function of the fixed nuclear coordinates R Ekin = kinetic energy of the electrons Eelec-nuc= the attractive interaction between the electrons and the nuclei Eelec-elec= the electron-electron repulsion energy

Decoupling of the electronic motion from the nuclear motion is known as the Born-Oppenheimer approximation introduced by J. Robert Oppenheimer and Max Born.

A further difficulty was expected the last term of eq. (1) electron-electron repulsion. Without this term, it is feasible to utilize the strategy for partition of variables to tackle the Schrödinger equation independently for every electron, except this isn't conceivable when the term is inclusive.

The standard estimation, created by Hartree and Fock, to get rid of this problem is to expect that every electron moves in the average field because of the nuclei and other electrons. The first Hartree strategy communicates the aggregate wave function of the framework as a result of one electron orbitals. In the Hartree-Fock technique, the wave function is an anti-symmetrized determinantal product of one-electron orbitals. Schrodinger's equation is changed into an arrangement of Hartree Fock conditions. The Hartree-Fock guess is likewise known at the self- consistent field (SCF) strategy which starts with a set of approximate orbitals for all the electrons in the molecule. One electron is chosen, and the potential in which it moves is calculated by freezing the distribution of all the other electrons and treating their averaged distribution as the centrosymmetric source of potential. The Schrodinger equation is solved for this potential, which provides a new orbital for it, the procedure is continual for all the other electrons in the system. At the completion of one cycle, there are new orbitals from the original set. The process is repeated until there is little or no change in the orbitals. The square of the atomic orbitals gives the probability density. Usually, molecular orbitals are expressed as linear combinations of atomic orbitals (LCAO), the sum of atomic orbitals centered on each nucleus.

Due to the central field approximation, the energies from HF counts are constantly more than the exact energy and tend to a limiting value called the Hartree-Fock limit as the basis set is improved. Inside HF hypothesis the possibility of finding an electron at some point around an atom determined by the distance from the nucleus but not the distance to the other electrons. A number of types of calculations begin with an HF calculation and various sorts of computations start with an HF calculation and then correct for correlation.

Some of these methods are Moller-Plesset perturbation theory (MPn, where n is the order of correction), configuration interaction (CI), coupled cluster theory (CC), the generalized valence bond (GVB) method, multi-configurational self-DOI: 10.48175/IJARSCT-24756

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consistent field (MCSCF), and Density Functional theory (DFT)at that point amend for connection. Some of these strategies are Moller-Plesset annoyance hypothesis (MPn, where n is the request of redress), the summed up valence bond (GVB) strategy, multi-configurational self-consistent field (MCSCF), setup collaboration (CI), and coupled group hypothesis (CC) and Density Functional hypothesis (DFT).

In recent years Density practical hypothesis (DFT) has turned out to be extremely popular. This is supported by the pragmatic observation that it is less computationally exhaustive than other methods. The preface behind DFT is that the vitality of a particle can be resolved from the electron density rather than a wave function. This hypothesis began with a hypothesis by Hoenberg and Kohn that expressed this was conceivable. The first hypothesis connected just to finding the ground-state electronic energy of a molecule. A practical claim of this theory was developed by

Kohn and Sham who framed a method similar in structure to the Hartree-Fock method. In general, ab initio designs give very good qualitative outcomes and can yield increasingly precise quantitative results as the molecules chosen become smaller. The benefit of ab initio methods is that they eventually converge to the exact solution once all the approximations are made adequately small in magnitude.

Semi empirical calculations are set up with the same general structure as a HF calculation in that they have a wave function and Hamiltonian. Generally, the core electrons are not encompassed in the calculation and only a minimal basis set is used. Also, some of the two electron integrals are omitted. In order to rectify the errors introduced by omitting part of the calculation, the method is parameterized. Parameters to estimate the omitted values are obtained by getting the outcomes to experimental data or ab initio calculations. Often, these parameters replace some of the integrals that are excluded. The only advantage of semi empirical calculations are that they are much quicker than ab initio calculations. The shortcoming of semi empirical calculations is that the results can be uneven and fewer properties can be predicted reliably



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Advantages:

One important benefit of DFT is that DFT scales three dimensionally, or as N3, (N = number of basis functions). On the other hand Ab-initio methods, scale as N4. Hence DFT calculations are slightly faster with enhanced accuracy. DFT includes some component of electron correlation for much the same computational cost as HF methods. It is a highly efficient way of performing a more advanced calculation of the system. DFT can also perform calculations on transition metals that is not possible with ab-initio methods.

Disadvantages:

The computational chemist must make decisions about which DFT method or functional and basis set to use for a particular application. For example, the BLYP the method is considered by some to be appropriate for transition metal applications, but not for all organic compounds.

III. APPLICATION OF QUANTUM CHEMICAL METHODS IN GEOMETRY OPTIMIZATION

Geometry Optimization is a process that tries to find the configuration of minimum energy of the molecule. A sensible starting point for geometry optimization is to use experimental data. The energy and wave functions are computed for the initial guess of the geometry, which is then modified iteratively until (I) an energy minimum has been identified and (II) forces within the molecules are zero. This can often be difficult for non-rigid molecules, where there may be several energy minima, and some effort may be essential to find the global minimum. But in those cases where molecules have unknown or unconfirmed structures, geometry optimization can also be used to locate minima on a potential energy surface (PES).

An input geometry is provided for geometry optimization and the calculation proceeds to move across the PES. At each point the energy, as well as gradient, are calculated and the distance with the direction of the next step are determined. The force constants are generally estimated at each point and these constants specify the curvature of the surface at that point; this provides supplementary information useful to determining the next step. Convergence criteria about the forces at a given point and the displacement of the next step determine whether a stationary point has been found. To determine whether the geometry optimization has found a minimum or a transition state (TS), it is required to perform frequency calculations. A TS is a point that links two minima on the PES and is characterized by one imaginary frequency. The eigenvector from the Hessian force constant matrix determines the nature of the imaginary frequency and indicates a possible reaction coordinate. A minimum structure will have no imaginary frequencies.

IV. METHODS FOR MOLECULAR ELECTRONIC HYPERPOLARIZABILITY CALCULATIONS

Most common methods currently implemented are three methods-the finite field, sum-over-states (SOS), and timedependent Hartree-Fock methods-encompass the vast majority of NLO property calculations being performed today and are implemented in several readily available molecular orbital computer programs

Finite Field Method

It is the simplest method for obtaining nonlinear optical properties of molecules. This method was first used by Cohen and Roothaanzs to calculate atomic polarizabilities at the Hartree- Fock level.

Main advantages of finite field method: -

(1) Easy to implement, and

(2) Applied to a wide range of quantum mechanical methods.

Disadvantages of the finite field method: -

It is limited to static field therefore not give values directly related to most experiments.

Sum-Over-States Method

The most familiar expressions for obtaining nonlinear optical properties are the expressions derived from timedependent perturbation theory. This procedure is straightforward and has been described in detail equations can be used to obtain frequency-dependent properties.

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V. GRAPHICAL USER INTERFACE FOR GAUSSIAN 09 - GAUSS VIEW

Gauss view is a reasonable, full-featured graphical user interface for Gaussian 09[9]. With the help of Gauss view, one can prepare input for submission to Gaussian and to examine graphically the output that Gaussian produces. The first step in producing a Gaussian input file is to build the desired molecule. The bond lengths, bond angles, and dihedral angles for the molecule will be used by Gauss view to write a molecular structure for the calculation. Gauss view incorporates an excellent Molecule Builder. One can use it to rapidly sketch in molecules and examine them in three dimensions. Molecules can be built by atom, ring, group. Gauss view

is not integrated with the computational the module of Gaussian, but rather is a front-end or back-end processor to aid in the use of Gaussian. Gauss view can graphically display a variety of Gaussian calculation results, including the following

- Molecular orbitals
- Atomic charges
- Surfaces from the electron density, electrostatic potential.
- Surfaces can be colored by a separate property.
- · Animation of the normal modes corresponding to vibrational frequencies.
- Animation of the steps in geometry optimizations, potential energy surface scans.

Quantum chemical calculations have been shown to be useful in the description of the relationship between the electronic structure of the systems and its NLO response. The computational approach allows the determination of molecular NLO properties as an inexpensive way to design molecules by analyzing their potential before synthesis and to determine high-order hyperpolarizability tensors of molecules [10]. The polarizability (α), characterizes the ability of an electric field to distort the electronic distribution of a molecule. Higher order polarizability (hyperpolarizabilities β , γ) which describes the non-linear response of atoms and molecules. They are related to a wide range of phenomena from non-linear optics to intermolecular forces, such as the stability of chemical bonds, as well as, the conformation of molecules. The elements of these tensors from derivatives of the dipole moment with respect to the electric field and the first hyperpolarizability is a third rank tensor that can be described by a $3 \times 3 \times 3$ matrix. It strongly depends on the method and basis set used. The 27 components of the 3D matrix can be reduced to ten components because of the Kleinman symmetry [11]. The matrix can be given in the lower tetrahedral format. It is obvious that the lower part of the $3 \times 3 \times 3$ matrixes is tetrahedral. The components of β are defined as the co-efficient in the Taylor series expansion of the energy in the external electric field. When the external electric field is weak and homogeneous, this expansion becomes:

$$\mathbf{E} = \mathbf{E}^{0} - \boldsymbol{\mu}_{\alpha} f_{\alpha} - \frac{1}{2\alpha_{\alpha\beta}F_{\alpha}F_{\beta}} - f \frac{1}{6\beta_{\alpha\beta\gamma}F_{\alpha}F_{\beta}F_{\gamma}} \dots \dots (2)$$

where E° is the energy of the unperturbed molecules, $F\alpha$ is the field at the origin, $\mu\alpha$, $\alpha\alpha\beta$ and $\beta\alpha\beta\gamma$ are the components of dipole moment, polarizability, and the first hyperpolarizabilities respectively. The equations for calculating the magnitude of total static dipole moment (μ), the mean polarizability (α 0), the anisotropy of the polarizability ($\Delta\alpha$) the mean first hyperpolarizability (β 0) and static second hyperpolarizability (γ), using the x, y, z components from Gaussian 09W output are defined as follows

The strength of optical response depends on the electrical properties of the whole material, which for molecules can be related to the polarizability (α , linear response) and hyperpolarizabilities (β , γ , etc. nonlinear responses). The static second-order polarizability or first hyperpolarisability (β) and its related properties for NLOphores were calculated on the basis of the finite-field approach

[12] The equations for calculating the magnitude of total static dipole moment (μ), the mean polarizability (α 0), the anisotropy of the polarizability ($\Delta \alpha$) the mean first hyperpolarizability (β 0) and static second hyperpolarizability (γ), using the x, y, z components from Gaussian 09W output are defined as follows .

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The total static dipole moment μ is expressed as:

$$\mu = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2} \dots \dots (3)$$

The isotropic polarizability can be calculated from the trace of the polarization tensor,

$$\alpha_0 = \frac{(\alpha_{xx} + \alpha_{yy} + \alpha_{zz})}{3} \dots \dots \dots (4)$$

Anisotropy of the polarizability $\Delta \alpha$ is expressed by

$$\Delta \alpha = 2^{-1/2} \left[(\alpha_{xx} + \alpha_{yy})^2 + (\alpha_{zz} + \alpha_{xx})^2 + 6\alpha_{xx}^2 \right] \dots \dots (5)$$

The mean first polarizability $(\beta 0)$ is expressed by

where, βx , βy , and βz are the components of the second order polarizability tensor along the x, y and z axis. The equation for mean second hyperpolarizability (γ) is

$$\gamma = \frac{1}{5} [(\gamma_{xxxx} + \gamma_{yyyy} + \gamma_{zzzz}) + 2(\gamma_{xxyy} + \gamma_{yyzz} + \gamma_{zzxx})].....(7)$$

The fundamental limits of NLO response for the push-pull chromophores are obtained by the limiting theory proposed by Kuzyk[13,14]

The limit for β^* is obtained from eq.8in different solvents using their respective refractive indices (n).

$$\beta_{2L}^{*SR} \le {}^{4}\sqrt{3} \left(\frac{n^{2}+2}{3}\right)^{3} \left(\frac{e\hbar}{\sqrt{m}}\right)^{3} \frac{N^{3/2}}{E_{10}^{7/2}}$$
(8)

e and m are the charge and mass of the electron. $\hbar = h/2\pi$.

Similarly, the limit for the second order hyperpolarizability (γ) can be estimated by eq. 9 [15,16] The γ values have two possible fundamental limits for the i.e. negative limit which is for a centrosymmetric molecule and positive limit for an asymmetric molecule.

$$-\frac{e^4\hbar^4}{m}\left(\frac{N^2}{E_{10}^5}\right) \le \gamma \le 4 \frac{e^4\hbar^4}{m}\left(\frac{N^2}{E_{10}^5}\right) \tag{9}$$

In D- π -A organic molecules generally, vibrations are strongly coupled with conjugated electrons in the system. Hence along with the electronic transitions, the vibrational transitions play important role in determining the NLO properties. The coupling between the electronic polarization and vibration leads to a considerable vibrational contribution to the overall NLO response[17]. In this context, the DFT is a very good computational tool to study the vibrational contribution to polarizability and hyperpolarizabilities of NLO phores [18,19].

VI. CONCLUSION

This article elaborates recent advances in computational strategies for estimating NLO properties, highlighting their strengths, limitations, and applications.

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