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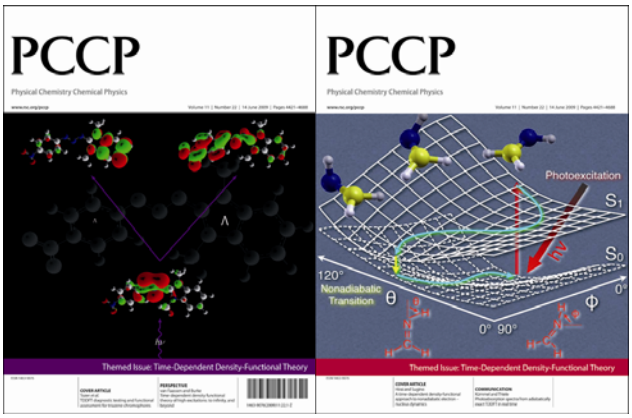
Time-Dependent Density-Functional Theory



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Miguel A. L. Marques and Angel Rubio

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Phys. Chem. Chem. Phys., 2009
DOI: 10.1039/b908105b

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A new generalized Kohn–Sham method for fundamental band-gaps in solids
Helen R. Eisenberg and Roi Baer, *Phys. Chem. Chem. Phys.*, 2009
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Time-dependent density-functional theory

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In spite of the tremendous effort focused over the years, the first-principles theoretical description of the interaction of molecules with time-dependent electromagnetic fields is still a challenging problem. If fact, we are still lacking a definitive and systematic methodology, capable of bridging the different spatial and time scales that are relevant for the description of light-induced processes in nanostructures, biomolecules and extended systems with predictive power. Time-dependent density-functional theory (TDDDFT) has repeatedly shown in the last decade its usefulness when attempting this challenge. The reason is the unparalleled balance between the computational load that it requires and the accuracy that it provides. The growing interest that TDDFT has been creating in the scientific community can be clearly measured by the exponential growth on the number of articles published in this field (similarly to what happened to standard density functional theory twenty years ago), and by the number of high-level scientific meetings focusing on TDDFT.

The foundations of modern TDDFT were laid in 1984 by Runge & Gross, who derived a Hohenberg–Kohn-like theorem for the time-dependent Schrödinger equation. The scope of this generalization of ground-state density functional theory included the calculation of photoabsorption spectra or, more generally, the interaction of electromagnetic fields with matter, as well as the time-dependent description of scattering experiments (which was actually the original motivation of Runge & Gross).

Today, the use of TDDFT is increasing in all areas where interactions are important but the direct solution of the Schrödinger equation is too demanding. It is fast becoming one of the tools of choice to get accurate and reliable predictions for excited-state properties in solid state physics, chemistry and biophysics, both in the linear and non-linear regimes. This interest has been motivated by the recent developments of TDDFT and include the description of photo-absorption cross section of molecules and nanostructures, electron-ion dynamics in the excited state triggered by either weak or intense laser fields, van der Waals interactions, development of new functionals coping with memory and non-locality effects, applications to biological systems (chromophores), transport phenomena, optical spectra of solids and low-dimensional structures (as nanotubes, polymers, surfaces, *etc.*).

Other new and exciting applications are beginning to emerge, from ground-state energies extracted from TDDFT to transport through single molecules, to high-intensity lasers and non-equilibrium phenomena, to non-adiabatic excited-state dynamics, to low-energy electron scattering. Present approximations to the elusive exchange–correlation functional work extremely well for many of these properties, but occasionally fail for others. Thus, the search for more accurate and reliable approximations will continue, and over time, should attain the same maturity as in present ground-state DFT.

It is the purpose of this themed issue—on the 25th anniversary of TDDFT—to overview, by presenting several examples, some of the capabilities and successes of this approach, at the same time highlighting its current limits and deficiencies. The present volume contains a collection of the very recent developments of TDDFT: from fundamentals to complex applications of technological relevance. The contributors have recognised reputation in the field and the present compilation should serve as reference for researchers, complementing and updating the available comprehensive review of the developments of TDDFT: *Time-Dependent Density-Functional Theory*, ed. M. A. L. Marques, C. Ullrich, F. Nogueira, A. Rubio and E. K. U. Gross, *Lecture Notes in Physics* **706**, Springer Verlag, Berlin, 2006.

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