



Time-Dependent Density Functional Theory (Lecture Notes in Physics)

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The year 2004 was a remarkable one for the growing field of time-dependent density functional theory (TDDFT). Not only did we celebrate the 40th anniversary of the Hohenberg-Kohn paper, which had laid the foundation for ground-state density functional theory (DFT), but it was also the 20th anniversary of the work by Runge and Gross, establishing a firm footing for the time-dependent theory. Because the field has grown to such prominence, and has spread to so many areas of science (from materials to biochemistry), we feel that a volume dedicated to TDDFT is most timely. TDDFT is based on a set of ideas and theorems quite distinct from those governing ground-state DFT, but employing similar techniques. It is far more than just applying ground-state DFT to time-dependent problems, as it involves its own exact theorems and new and different density functionals. Presently, the most popular application is the extraction of electronic excited-state properties, especially transition frequencies. By applying TDDFT after the ground state of a molecule has been found, we can explore and understand the complexity of its spectrum, thus providing much more information about the species. TDDFT has a especially strong impact in the photochemistry of biological molecules, where the molecules are too large to be handled by traditional quantum chemical methods, and are too complex to be understood with simple empirical frontier orbital theory.

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