Time-dependent density functional theory: An overview

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This talk will be an overview of the state-of-the-art of TDDFT. This formalism has been very successful in going beyond ground-state DFT to extract electronic excitations of molecules and clusters, and has become a routine tool in quantum chemistry. Applications to bulk systems have been slower, due to problems with the locality of common density functionals.

I hope to quickly discuss: basic ideas and theorems, linear response theory, applications and performance, complications for solids, new functionals, and new applications, including molecular electronics.

For background, some recent references include:

Time-dependent density functional theory, edited by M. Marques, C.A. Ullrich, F. Noguiera, A. Rubio, K. Burke, and E.K.U. Gross (Springer, Heidelberg, 2006).
(http://www.springer.com/east/home/physics?SGWID=5-10100-22-173664005 detailsPage=ppmmedia)

and

Time-dependent density functional theory: Past, present, and future,
K. Burke, J. Werschnik, and E.K.U. Gross, J. Chem. Phys. 123, 062206 (2005)