

QED-Chemistry and Materials: A First principles modeling of Light-Matter interactions within QED-TDDFT

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Computer simulations that predict the light-induced change in the physical and chemical properties of complex systems, molecules, nanostructures and solids usually ignore the quantum nature of light. We have recently shown how the effects of the photons can be properly included in such calculations. The basic idea is to treat the full QED system of particles and photons as a quantum fluid. Here the particles are represented by a charge current, and the photons by a classical electromagnetic field that acts on the current in a very complex manner. This study opens up the possibility to predict and control the change of material properties due to the interaction with light particles from first principles .

Here we will review the recent advances within density-functional a schemes to describe spectroscopic properties of complex systems with special emphasis to modeling time and spatially resolved electron spectroscopies We will discuss the theoretical approaches developed in the group for the characterization of matter out of equilibrium, the control material processes at the electronic level and tailor material properties, and master energy and information on the nanoscale to propose new devices with capabilities. Our goal is to provide a detailed, efficient, and at the same time accurate microscopic approach for the ab-initio description and control of the dynamics of decoherence and dissipation in quantum many-body systems. This theoretical framework provides a new way to control and alter chemical reactions in complex systems, direct the movement of electrons, selectively trigger physico-chemical processes, and create new state of mater

References:

- [1] Atoms and Molecules in Cavities: From Weak to Strong Coupling in QED Chemistry, J. Flick, M. Ruggenthaler, H. Appel, A. Rubio, Proceedings of The National Academy of Sciences of The United States of America 114, 3026–3034 (2017)
- [2] Kohn-Sham Approach to Quantum Electrodynamical Density Functional Theory: Exact Time-Dependent Effective Potentials in Real Space J. Flick, M. Ruggenthaler, H. Appel, A. Rubio, Proceedings of The National Academy of Sciences of The United States of America 112 15285-15290 (2015)
- [3] Optimized Effective Potential for Quantum Electrodynamics Time-Dependent Density Functional Theory C. Pellegrini, J. Flick, I. V. Tokatly, H. Appel and A. Rubio Physical Review Letters 115, 093001 (2015)
- [4] Quantum Electrodynamics Density-Functional Theory: Bridging Quantum Optics and Electronic-Structure Theory M. Ruggenthaler, J. Flick, C. Pellegrini, H. Appel, I. V. Tokatly, A. Rubio, Physical Review A 90 012508-1,26 (2014)