

**Thursday, 3<sup>rd</sup> May 2018, 17:00**

*Campus Schenefeld, main building (XHQ) room E1.172*

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## How photons change the properties of matter

In this talk I will present a brief overview of how the standard description of quantum chemistry and material sciences have to be adapted when photons become important in correlated light-matter problems [1,2], and possible ways to tackle such situations with ab-initio methods [3-6]. I will highlight that quantum-electrodynamical density-functional theory [3,5], an exact quantum-fluid reformulation of quantum electrodynamics, is a natural framework to determine equilibrium as well as non-equilibrium properties of coupled matter-photon systems, such as new composite (fermionic/bosonic) quasi-particles [1,2], changes in the Born-Oppenheimer surfaces and in chemical reactions [1,2], the emergence of collective effects or changes in the intrinsic lifetimes [7], from first principles.

[1] M. Ruggenthaler, N. Tancogne-Dejean, J. Flick, H. Appel, and A. Rubio, "From a quantum-electrodynamical light-matter description to novel spectroscopies", *Nature Reviews Chemistry* 2, 0118 (2018).

[2] J. Flick, M. Ruggenthaler, H. Appel, and A. Rubio, "Atoms and molecules in cavities, from weak to strong coupling in quantum-electrodynamics (QED) chemistry", *Proceedings of the National Academy of Sciences* 114 (12), 3026-3034 (2017).

[3] M. Ruggenthaler, J. Flick, C. Pellegrini, H. Appel, I.V. Tokatly, and A. Rubio, "Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory" *Physical Review A* 90 (1), 012508 (2014).

[4] J. Flick, M. Ruggenthaler, H. Appel, and A. Rubio, "Kohn-Sham approach to quantum electrodynamical density-functional theory: Exact time-dependent effective potentials in real space", *Proceedings of the National Academy of Sciences* 112 (50), 15285-15290 (2015).

[5] M. Ruggenthaler, "Ground-state quantum-electrodynamical density-functional theory", arXiv:1509.01417 (2017).

[6] C. Schaefer, M. Ruggenthaler, and A. Rubio, "Insights from ab-initio non-relativistic quantum electrodynamics: Bridging quantum chemistry and quantum optics", arXiv:1804.00923 (2018).

[7] J. Flick, D.M. Welakuh, M. Ruggenthaler, H. Appel, and A. Rubio, "Light-Matter Response Functions in Quantum-Electrodynamical Density-Functional Theory: Modifications of Spectra and of the Maxwell Equations", arXiv:1803.02519 (2018).

**Host: Evgeny Gorelov**