CFEL SCIENCE

SEMINAR

16th February 2022 - 2:00 p.m.

Virtual meeting room in ZOOM (ID: 895 1951 2902 / PW: 925239)

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Towards a detailed understanding of (strong) light-matter coupling effects

In the last decade a host of seminal experimental results have demonstrated that properties and dynamics of molecules and solids can be modified and controlled by coupling strongly to the electromagnetic field of a photonic environment, e.g. an optical cavity. For a detailed understanding of such changes it becomes necessary to use first-principles approaches to strong light-matter interactions.

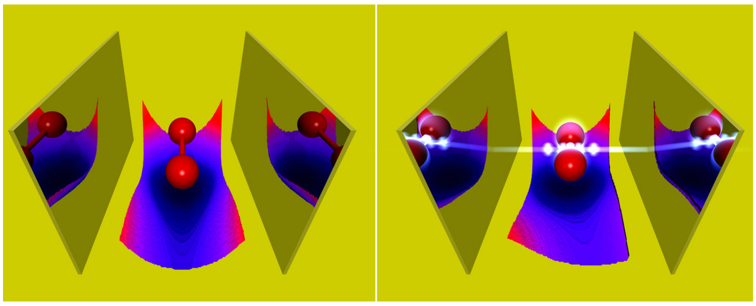
In this talk I will discuss the fundamental setting for such ab-initio methods, the Pauli-Fierz quantum field theory in Coulomb gauge, introduce quantum-electrodynamical density-functional theory as an efficient and accurate simulation technique [1,2] and highlight novel effects that become accessible. Among others I demonstrate how chemical properties can be modified, how collective strong coupling can induce strong local modifications and how long-standing problems can be resolved when including the photonic degrees of freedom from first principles [3].

References

[1] M. Ruggenthaler *et al.*, “From a quantum-electrodynamical light–matter description to novel spectroscopies,” *Nat. Rev. Chem.* 2, 0118 (2018).

[2] M. Ruggenthaler *et al.*, “Quantum-electro-dynamical density-functional theory: Bridging quantum optics and electronic-structure theory,” *Phys. Rev. A* 90, 012508 (2014).

[3] V. Rokaj *et al.*, “Quantum electrodynamical Bloch theory with homogeneous magnetic fields,” *Phys. Rev. Lett.* 123, 047202 (2019).



The properties of a molecule, e.g., the equilibrium bond length, can be controlled by modifying the vacuum field inside an optical cavity. On the right-hand side the modifications of the vacuum field achieve strong light-matter coupling.

Host: Robin Santra – CFEL-DESY Theory Division