



# Sommerfeld Theory Colloquium

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Quantum Electrodynamics Density functional theory (QEDFT):  
cavity quantum materials engineering

An appealing and challenging route towards engineering materials with specific properties is to find ways of designing or selectively manipulate materials, especially at the quantum level. We will provide an overview of how well-established concepts in the fields of quantum chemistry and materials have to be adapted when the quantum nature of light becomes important. We will pursue the question whether it is possible to create these new states of materials as groundstates of the system. To this end we will show how the emerging (vacuum) dressed states resembles Floquet states in driven systems. A particular appeal of light dressing is the possibility to engineer symmetry breaking which can lead to novel properties of materials, e.g. coupling to circularly polarized photons leads to local breaking of time-reversal symmetry enabling the control over a large variety of materials properties (e.g. topology). We show that the new quantum electrodynamics density-functional formalism (QEDFT) can account for those effects. We illustrate the realisation of those ideas in molecular complexes and 2D materials.

Wednesday, 24 January 2024, 16:15h, Room A348, Theresienstr. 37/III

Dr. C. Schilling