Chez Pierre

Presents ...

Monday, March 3rd, 2025

12:00 pm -1:00 pm

Duboc Room – 4-331

Chez Pierre Seminar

Angel Rubio, Max Planck Institute

"Harnessing Cavity Vacuum Fluctuations for Quantum Materials Engineering: a QEDFT Framework"

A major challenge in computational physics is developing accurate and efficient theories for non-equilibrium, light-driven phenomena and emerging states of matter. Time-Dependent Density Functional Theory (TDDFT) has been instrumental in simulating light-induced modifications in complex systems. Extending this, Quantum Electrodynamics Density-Functional Theory (QEDFT) provides a first-principles framework to predict and manipulate ordered phases in strongly coupled light-matter hybrids, or polaritons, enabling phenomena like photon-mediated superconductivity and optically driven topological states. This burgeoning field, Cavity Materials Engineering, leverages strong electron-photon coupling to design novel quantum states. A key paradigm shift lies in harnessing vacuum quantum fluctuations to alter material ground states without populating photon modes. Unlike conventional polaritonic physics, this "dark" regime enables ground-state quantum phase transitions driven solely by vacuum fluctuations, unlocking profound material transformations. Grounded in non-relativistic QED, QEDFT unifies light-matter coupling with electronic properties, providing a robust framework for engineering quantum materials. This approach opens exciting opportunities to design and control quantum materials, advancing our understanding of matter at the intersection of light and quantum phenomena.

Some relevant recent references

•Engineering quantum materials with chiral optical cavities , H. Hübener, U. D. Giovannini, C. Schäfer, J. Andberger, M. Ruggenthaler, J. Faist, and A. Rubio Nature Materials 20, 438-442 (2021)

•Cavity engineered phonon-mediated superconductivity in MgB2 from first principles quantum electrodynamics, I-T. Lu, Dongbin Shin, Mark Kamper Svendsen, Hannes Hübener, Umberto De Giovannini, Simone Latini, Michael Ruggenthaler, Angel Rubio, Proceedings of the National Academy of Science USA (PNAS) 121, e2415061121 (2024)

•Controlling the magnetic state of the proximate quantum spin liquid α-RuCl3 with an optical cavity, Emil Vinas Boström, Adithya Sriram, Martin Claassen, Angel Rubio, npj Computational Materials 9, 202 (2023)

•The ferroelectric photo ground state of SrTiO3: Cavity materials engineering, S. Latini, D. Shin, S. A. Sato, C. Schäfer, U. D. Giovannini, H. Hübener, and A. Rubio PNAS 118, e2105618118 (2021)

•Understanding polaritonic chemistry from ab initio quantum electrodynamics, M. Ruggenthaler, D. Sidler, A. Rubio, Chemical Reviews 123, 11191 (2023)

•Theory of quantum light-matter interaction in cavities: Extended systems and the long wavelength approximation, Mark Kamper Svendsen, Michael Ruggenthaler, Hannes Hübener, Christian Schäfer, Martin Eckstein, Angel Rubio, Simone Latini arXiv: arXiv:2312.17374

•Cavity Spectroscopy for Strongly Correlated Systems, Lukas Grunwald, Emil Viñas Boström, Mark Kamper Svendsen, Dante M. Kennes, Angel Rubio, arXiv:2410.21515