Chemistry in Quantum Cavities: Exact Results in Thermal Equilibrium and Modified Dissociation

Presenter:
Dominik Sidler
(Max Planck Inst Structure & Dynamics of Matter)

Authors:
Dominik Sidler
(Max Planck Inst Structure & Dynamics of Matter)

Michael Ruggenthaler
(Max Planck Inst Structure & Dynamics of Matter)

Heiko Appel
(Max Planck Inst Structure & Dynamics of Matter)

Angel Rubio
(Max Planck Inst Structure & Dynamics of Matter)

In recent years tremendous progress in the field of light-matter interactions has unveiled that strong coupling to an optical cavity can modify chemistry substantially. However, many fundamental questions of chemistry in cavities remain open today. This is also due to a lack of exact results that can be used to validate and benchmark approximate approaches. We provide, to our knowledge, the first exact numerical results for the Pauli-Fierz Hamiltonian of a three-body systems in 3D, coupled to one effective cavity mode. This allows us to investigate the reliability of the ubiquitous Jaynes-Cummings model not only for electronic but also for the case of ro-vibrational transitions of He, H_2^+ and HD+. We show the emergence of new bound polaritonic states beyond the dissociation energy limit of H_2^+ and we demonstrate the modification of chemical properties under thermal equilibrium conditions.

[1] Sidler, D.; Ruggenthaler, M.; Appel, H.; Rubio, A. *J. Phys. Chem. Lett.* 2020 (accepted), 10.1021/acs.jpclett.0c01556

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