

## MO 11: Poster – Polaritonic Effects in Molecular Systems (joint session MO/Q)

Time: Tuesday 14:00–16:00

Location: Tent

MO 11.1 Tue 14:00 Tent

**Modifying the electronic properties of the topological systems with cavity** — ●SABER ROSTAMZADEH, REMI AVRILLER, CLEMENT DUTREIX, and FABIO PISTOLESI — Laboratoire Ondes et Matière d'Aquitaine, Université de Bordeaux, France

Topological systems exhibit fascinating electronic applications due to their distinctive edge and zero-mode states. A central question is how these states interact with various environments, such as intense light. Similarly, hybrid quantum systems containing a few electrons, such as quantum dots, serve as valuable models for engineering topological electronic states. These systems have also garnered significant interest in cavity quantum electrodynamics (cavity QED) for their potential to achieve ultrastrong light-matter interactions. Their simplified architectures offer significant enhancements and optimizations in electron-photon coupling. In this study, we investigate modifications in electronic transport within single and double quantum dot arrays placed inside a cavity.

MO 11.2 Tue 14:00 Tent

**Vibrational dynamics of individual oscillators under Vibrational Strong Coupling** — ●HELENA POULOSE<sup>1</sup>, MATHIS NOELL<sup>2</sup>, YANNIK PFEIFER<sup>1</sup>, TILL STENSITZKI<sup>1</sup>, CARSTEN HENKEL<sup>2</sup>, WOUTER KOOPMAN<sup>2</sup>, and HENRIKE MÜLLER-WERKMEISTER<sup>1</sup> — <sup>1</sup>Institut für Chemie, Universität Potsdam, Germany — <sup>2</sup>Institut für Physik und Astronomie, Universität Potsdam, Germany

The novel field of polariton chemistry opens up a way to tune material properties and steer chemical reactions by manipulating quantum light-matter interactions. Fabry-Perot cavities can be constructed to confine electromagnetic field, allowing the light mode to strongly couple with vibrational transitions of molecules, generating quasi light-matter states, characterised by vacuum rabi splitting. However the underlying mechanism behind how it effects the reaction dynamics is not completely understood. Combining Ultrafast nonlinear spectroscopy with Strong coupling could provide insights to how the energy distribution changes when these delocalized hybrid states are formed. Experiments of vibrational dynamics can possibly provide valuable insights into the fundamental mechanisms of polaritons and how polaritons might modulate Chemistry. Here we report on our a) cavity design and characterisation, b) static polariton spectra supported by theory and c) first attempts in performing nonlinear IR and 2DIR spectra of organic compounds, like Benzaldehyde(C=O), under VSC in cavities. We aim to investigate vibrational lifetimes and energy transfer processes and examining how these depend on cavity and molecular properties.

MO 11.3 Tue 14:00 Tent

**Coherent state switching using vibrational polaritons in an asymmetric double-well potential** — ●LOÏSE ATTAL<sup>1</sup>, FLORENT CALVO<sup>2</sup>, CYRIL FALVO<sup>1,2</sup>, and PASCAL PARNEIX<sup>2</sup> — <sup>1</sup>Université Paris-Saclay, CNRS, Institut des Sciences Moléculaires d'Orsay, 91405 Orsay, France — <sup>2</sup>Université Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France

The quantum dynamics of vibrational polaritonic states arising from the interaction of a bistable molecule with the quantized mode of a Fabry-Perot microcavity is investigated using {a generic} asymmetric double-well potential as a simplified one-dimensional model of a reactive molecule. After discussing the role of the light-matter coupling strength in the emergence of avoided crossings between polaritonic states, we investigate the possibility of using these crossings to trigger a dynamical switching of these states from one potential well to the other. Two schemes are proposed to achieve this coherent state switching, either by preparing the molecule in an appropriate vibrational excited state before inserting it into the cavity, or by applying a short laser pulse inside the cavity to obtain a coherent superposition of polaritonic states. The respective influences of the dipole amplitude

and potential asymmetry on the coherent switching process are also discussed.

MO 11.4 Tue 14:00 Tent

**Chemical reaction rate of molecules in a cavity** — ●YANNIC JOSHUA BANTHIEN<sup>1</sup>, ABRAHAM NITZAN<sup>2</sup>, and MICHAEL THORWART<sup>1</sup> — <sup>1</sup>I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany — <sup>2</sup>Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA

We determine the reaction dynamics of N identical molecular systems, each represented by a particle in a double-well potential and each coupled to the same broadened mode of an optical cavity. Every reaction system is restricted to its lowest four energy eigenstates of the double well, forming a doublet-doublet system. A Markovian approximated master equation is set up following the Feynman-Vernon approach. It is constructed for the purpose of strong system-bath interaction. We solve for the time evolution of the quantum many-body system and extract the inter- and intra-well relaxation rates, leading to the chemical reaction rate. We study the impact of the common cavity mode on the reaction rate, determine the condition under which a Rabi splitting is found, and reveal emerging cooperative effects in the transfer rate.

MO 11.5 Tue 14:00 Tent

**Modifying Photoacids under Vibrational Strong Coupling** — ●SWATHI SWAMINATHAN<sup>1</sup>, JULIA BERGER<sup>2</sup>, GREGOR JUNG<sup>2</sup>, and THOMAS EBBESEN<sup>1</sup> — <sup>1</sup>University of Strasbourg, Strasbourg, France — <sup>2</sup>Saarland University, Saarbrücken, Germany

Vibrational strong coupling (VSC) between molecular transitions and cavity modes can significantly alter molecular properties and intermolecular interactions in the ground state. Here we explore the properties of photoacids,<sup>[1]</sup> which exhibit acidity in the excited state, and provide an ideal platform to explore the effects of VSC on their photo-physics. Photoacids typically exhibit characteristic fluorescence properties associated with the proton transfer from the solute to the solvent. Under cooperative VSC, we observe that this behavior is modified. This study shows that VSC can also affect excited-state properties, opening new avenues for understanding and controlling light-induced processes in molecular systems under strong coupling conditions.

[1] B. Finkler et al., Photochem. Photobiol. Sci. 2016, 15, 1544.

MO 11.6 Tue 14:00 Tent

**Vibrational strong coupling: a detailed analysis of the cavity tilt angle** — ●MATHIS NOELL<sup>1</sup>, HELENA POULOSE<sup>2</sup>, YANNIK PFEIFER<sup>2</sup>, TILL STENSITZKI<sup>2</sup>, WOUTER KOOPMAN<sup>1</sup>, HENRIKE MÜLLER-WERKMEISTER<sup>2</sup>, and CARSTEN HENKEL<sup>1</sup> — <sup>1</sup>Universität Potsdam, Institut für Physik und Astronomie — <sup>2</sup>Universität Potsdam, Institut für Chemie

Plasmonic chemistry is an emerging field that seeks to uncover new pathways for chemical reactions. One intriguing phenomenon in this domain is the strong coupling between a plasmonic cavity field and molecular excitations, resulting in the formation of hybrid polariton states. These hybrid states can modify potential energy surfaces and potentially tune material properties to benefit from enhanced reaction rates. To deepen our understanding of polariton dynamics, we investigate an analogous system where molecular vibrational resonances hybridize with an IR Fabry-Pérot cavity field mode. In this work, we present a detailed analysis of vibrational cavity strong coupling under angular variation, including the shift in polariton energy as the cavity is tilted. Additionally, we explore the polariton composition (Hopfield coefficients) and predict transmission, reflection, and absorption spectra. Our goal is to compare these theoretical results with pump-probe experiments, thereby contributing to a more comprehensive understanding of strong coupling dynamics.