# Symposium Polaritonic Effects in Molecular Systems (SYPE)

jointly organised by
the Molecular Physics Division (MO) and
the Quantum Optics and Photonics Division (Q)

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# Overview of Invited Talks and Sessions

(Lecture hall HS 1+2)

## Invited Talks

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|---|---|---|---|---|
| SYPE 1.1 | Tue | 11:00–11:30 | HS 1+2 | **Ab initio quantum electrodynamics: from microscopic details to thermodynamics** — •Michael Ruggenthaler |
| SYPE 1.2 | Tue | 11:30–12:00 | HS 1+2 | **Ultrafast coherent exciton dynamics mediated by field-matter couplings** — •Antonietta De Sio |
| SYPE 1.3 | Tue | 12:00–12:30 | HS 1+2 | **Open system dynamics for non-radiative transitions in molecules** — •Claudiu Genes |
| SYPE 1.4 | Tue | 12:30–13:00 | HS 1+2 | **Strong light-matter coupling: from self-hybridized polaritons to Casimir self-assembly** — •Timur Shegai |

## Sessions

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| SYPE 1.1–1.4 | Tue | 11:00–13:00 | HS 1+2 | **Polaritonic Effects in Molecular Systems** |

# SYPE 1: Polaritonic Effects in Molecular Systems

Time: Tuesday 11:00–13:00 Location: HS 1+2

**Invited Talk** SYPE 1.1 Tue 11:00 HS 1+2

**Ab initio quantum electrodynamics: from microscopic details to thermodynamics** — •Michael Ruggenthaler — Max-Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I will highlight how the microscopic details of an ab-initio quantum-electrodynamical description of matter can lead to changes in the thermodynamics. To elucidate this connection I will use different representative models from polaritonic chemistry and cavity materials engineering.

**Invited Talk** SYPE 1.2 Tue 11:30 HS 1+2

**Ultrafast coherent exciton dynamics mediated by field-matter couplings** — •Antonietta De Sio — Institut für Physik, Carl von Ossietzky Universität Oldenburg

Coupling electromagnetic radiation with matter is highly promising for tailoring optoelectronic and transport properties of functional materials, with potential applications ranging from photovoltaics to nanophotonics and quantum technologies. The underlying processes involve a complex interplay of electronic, vibrational, and photonic degrees of freedom and occur on ultrashort, few 100s-fs timescales, thus demanding techniques combining high time resolution and the ability to unravel couplings. Here, we present some recent results using broadband two-dimensional electronic spectroscopy to probe couplings and track their quantum dynamics. In halide perovskites, we demonstrate intra-exciton population oscillations driven by coherent phonon fields which behave essentially as arising from the coupling of excitons to a field mode in an off-resonant cavity [1]. In molecular aggregates deposited on a gold nanoslit array, where molecular excitons are collectively coupled to a spatially structured plasmonic field, we observe coherent oscillations due to plasmon-induced coherent exciton population transfer over mesoscopic distances [2]. Our results suggest strategies for controlling ultrafast coherent dynamics in functional materials. [1] Nguyen et al, Nature Comm. 14, 1047 (2023); [2] Timmer et al, Nature Commun. 14, 8035 (2023).

**Invited Talk** SYPE 1.3 Tue 12:00 HS 1+2

**Open system dynamics for non-radiative transitions in molecules** — •Claudiu Genes — TU Darmstadt, Darmstadt, and Max Planck Institute, Erlangen,Germany

Non-adiabatic molecular phenomena, arising from the breakdown of the Born-Oppenheimer approximation, govern the fate of virtually all photo-physical and photochemical processes and limit the quantum efficiency of molecules and other solid-state embedded quantum emitters. A simple and elegant description, the energy gap law, was derived five decades ago, predicting that the non-adiabatic coupling between the excited and ground potential landscapes lead to non-radiative decay with a quasi-exponential dependence on the energy gap. We revisit and extend this theory to account for crucial aspects such as vibrational relaxation, dephasing, radiative loss and most importantly, by considering higher order of non-adiabatic couplings beyond the constant case. We find closed analytical solutions allowing to decipher the mechanisms leading to non-radiative transitions. Our work establishes a connection between nanoscale quantum optics, open quantum system dynamics and non-adiabatic molecular physics and proposes an analytical approach to these processes.

**Invited Talk** SYPE 1.4 Tue 12:30 HS 1+2

**Strong light-matter coupling: from self-hybridized polaritons to Casimir self-assembly** — •Timur Shegai — Department of Physics, Chalmers University of Technology, 412 96, Gothenburg, Sweden

In this talk, I will give an overview of several nanophotonic systems that support polaritons, as well as demonstrate their potential usefulness in applications. I will start with transition metal dichalcogenides (TMDs) and discuss the concept of self-hybridization, a scenario in which both light and matter subparts in a polaritonic system are supported by the same (nano)structured material (1-4). We have recently demonstrated such self-hybridization in TMD nanostructures (1-4) and levitating water droplets (4-5). The latter is interesting, due to the abundance of water droplets in natural systems, including mists, fogs, and clouds. Furthermore, I will show that Fabry-Pérot resonators, one of the most important workhorses of nanophotonics, can spontaneously form in an aqueous solution of gold nanoflakes (6-8). This effect is possible due to the intricate balance between attractive Casimir-Lifshitz forces and repulsive electrostatic forces acting between the flakes.

(1) Nat. Commun., 11, 4604, (2020) (2) Laser & Photonics Rev., 17, 2200057, (2023) (3) Nat. Photon., 18, 751-757, (2024) (4) J. Chem. Phys., 154, 024701, (2021) (5) Phys. Rev. Lett., 132, 193804, (2024) (6) Nature, 597, 214-219, (2021) (7) Nat. Phys., 19, 271-278, (2023) (8) Sci. Adv., 10, eadn1825, (2024)