

## CAVITY-INDUCED MODIFICATION OF MOLECULES

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Organic molecules have long been recognized as a favorable type of emitter to achieve the strong-coupling regime, i.e., exciton-polariton formation, even at room temperature due to their large dipole moments and the stability (large binding energy) of Frenkel excitons. Strong coupling creates a paradigmatic hybrid quantum system with eigenstates that have mixed light-matter character, so-called polaritons. Traditionally, this has been used to achieve new functionalities in which polaritons are thought of as dressed photons, e.g., by exploiting exciton-exciton interaction to achieve interacting polaritons. However, over the last years, it has become clear that this regime also allows to significantly modify internal material properties and dynamics. Polariton formation leads to changes in the excited-state character and energy levels (i.e., potential energy surfaces) of the involved molecules, which can affect a wide range of properties, such as energy transport, photochemical reactions, and even thermally driven ground-state chemical reactions.

At the same time, organic molecules are highly complex material systems with a large number of nuclear (vibrational) degrees of freedom. Consequently, an accurate theoretical description of such systems faces a large amount of challenges: Fundamentally, electronic, nuclear, and (quantized) photonic degrees of freedom have to be treated on an equal footing both statically and dynamically. Typical experimental systems display ultrafast femtosecond-scale dynamics in their coupled photonic, electronic, and nuclear degrees of freedom due to room-temperature molecular dynamics and (typically) femtosecond-scale lifetimes of the cavity modes and plasmonic resonances employed as the photonic components of the polaritons. A theoretical description of these systems thus requires a combination of techniques from historically separate fields such as quantum optics, quantum chemistry, and ultrafast laser science.

I will give an overview over some effects observed in these systems, focusing on ways to observe and manipulate ultrafast dynamics in these systems, as well as different proposals for steering and catalyzing (photo)chemical reactions.

### References

- [1] J. Feist, J. Galego, F. J. Garcia-Vidal, *ACS Photonics*, 2018, **5**, 205.
- [2] J. Galego, F. J. Garcia-Vidal, and J. Feist, *Phys. Rev. Lett.*, 2017, **119**, 136001.
- [3] J. del Pino, F. A. Y. N. Schröder, A. W. Chin, J. Feist, F. J. Garcia-Vidal, *Phys. Rev. Lett.*, 2018, **121**, 227401.
- [4] C. Climent, J. Galego, F. J. Garcia-Vidal, J. Feist, *Angew. Chem. Int. Ed.*, 2019, **58**, 8698.
- [5] J. Galego, C. Climent, F. J. Garcia-Vidal, J. Feist, *Phys. Rev. X*, 2019, **9**, 021057.
- [6] R. Sáez-Blázquez, J. Feist, E. Romero, A. I. Fernández-Domínguez, F. J. García-Vidal, *J. Phys. Chem. Lett.*, 2019, **10**, 4252.
- [7] R. E. F. Silva, J. del Pino, F. J. García-Vidal, J. Feist, arXiv:1907.12607.
- [8] G. Groenhof, C. Climent, J. Feist, D. Morozov, J. J. Toppari, *J. Phys. Chem. Lett.*, 2019, 10.1021/acs.jpcclett.9b02192.