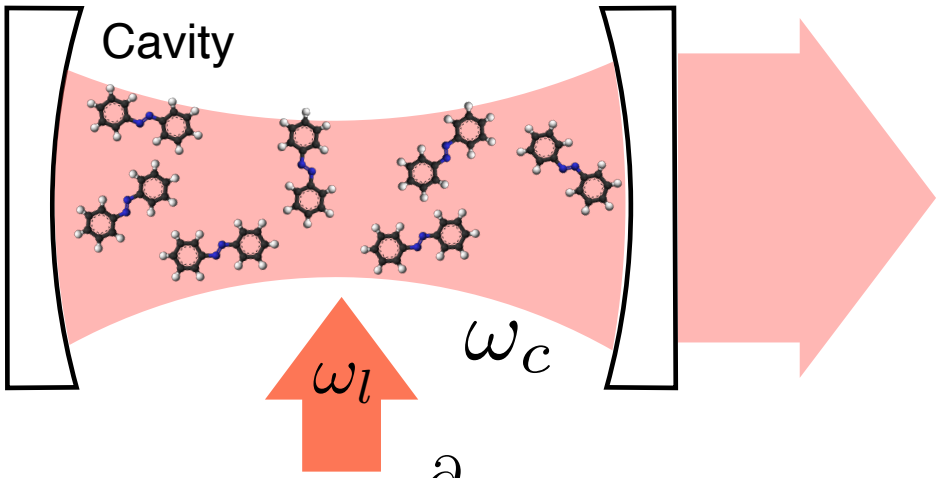
PhD position / *Promotionsstelle*

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Dynamical pathways of N-heteropolycycles in the strong light-matter coupling regime.

Description: A fully funded PhD position is available in the Theoretical Chemistry Group, Heidelberg University, within the recently extended SFB 1249 (*N-Heteropolyzyklen als Funktionsmaterialen*) for the period 2021-2024.

Possible starting date: Sommer semester 2021 or earlier.



$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$$

Aims and challenges: The strong light-matter coupling regime provides new opportunities to steer and control the structure and dynamics of molecular systems. Much progress in our group has been made towards simulating ultrafast dynamical processes in small molecules by quantum dynamics approaches [1-4]. The main goal of this project is to discover general strategies to modify the process of **singlet fission in N-heteropolycycles** by exploiting the coupling to the photonic modes of a resonance cavity. The project involves the usage and further development of state-of-the-art quantum dynamics methods, as well as close interaction with the experimental groups in the consortium.

Requisites:

- Master's degree (completed or about to complete) in related areas (e.g. chemistry or physics).
- Interest in the theory and numerical aspects of quantum dynamics.
- Interest in chemical dynamics and femto-chemistry.

Contact: Prof. Dr. Oriol Vendrell: (oriol.vendrell@uni-heidelberg.de)

SFB 1249 ***N*-Heteropolyzyklen als Funktionsmaterialien**

References:

[1] O. Vendrell; Coherent dynamics in cavity femtochemistry: Application of the multi-configuration time-dependent Hartree method. Chem. Phys **2018**
[2] O. Vendrell; Collective Jahn-Teller Interactions through Light-Matter Coupling in a Cavity; Phys. Rev. Lett. **2018**
[3] I. Ulusoy, J. Gomez, O. Vendrell; Modifying the Nonradiative Decay Dynamics through Conical Intersections via Collective Coupling to a Cavity Mode; JPCA **2019**
[4] I. Ulusoy, J. Gomez, O. Vendrell; Dynamics and spectroscopy of molecular ensembles in a lossy microcavity; J. Chem. Phys. **2020**