

# VISTA Seminar

## Seminar 28

**November 25, 2021**

**10:00 am – 11:30 am EST / 3:00 – 4:30 pm GMT / 4:00 pm – 5:30 pm  
Paris**

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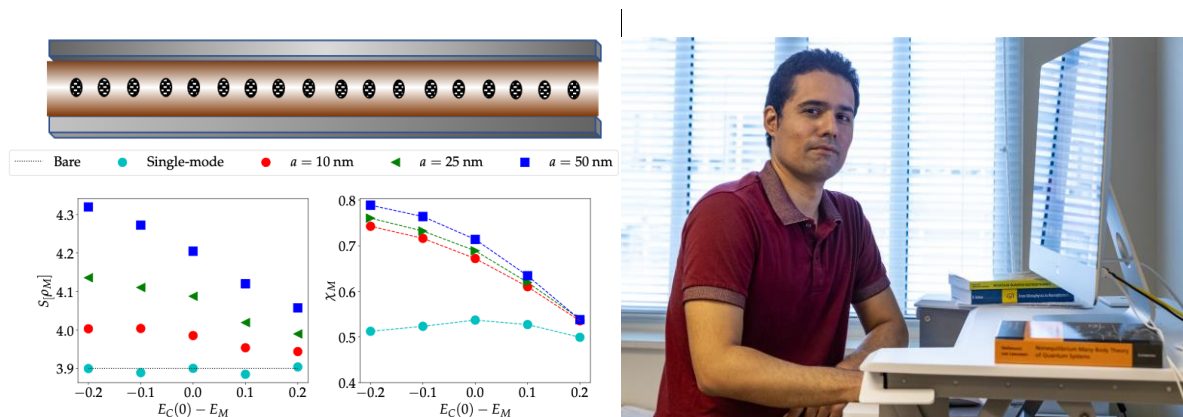
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## Spectral fluctuations and intermolecular energy transport in optical microcavities

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Optical cavities and metallic nanoparticles confine electromagnetic fields and enable new pathways to control physicochemical processes via strong light-matter interactions. In fact, recent experiments have shown that photonic and plasmonic materials may induce significant and sometimes unexpected changes to physical properties and reactivity of molecular systems.

In this talk, I will present the key results of our recent theoretical investigations of cavity-polariton effects on transport and spectral properties of disordered molecular ensembles hosted by a resonant 1D optical cavity (photonic wire). In light of these results, I will discuss strategies to maximize the influence of optical cavities on molecular materials, and show that widely employed minimal models fail to adequately describe photonic effects on certain local properties of chemical systems. I will conclude with a brief discussion of implications of our findings to future research on chemistry in optical microcavities.

## The SHARC-COBRAMM Interface for QM/MM Trajectory Surface Hopping Simulations with Arbitrary Couplings

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Trajectory Surface Hopping (TSH) is a widely used method to simulate nonadiabatic dynamics. By choosing an appropriate wavefunction representation, it can be extended to include various couplings, like spin-orbit couplings that drive intersystem crossing. Although the semi-classical nature of TSH allows the study of medium-large size systems, the inclusion of the environment surrounding a chromophore still requires the introduction of further approximations. One of the most successful ways to consider solvent and environmental effects is to apply a quantum mechanical/molecular mechanics (QM/MM) partition, treating the chromophore and its surrounding at two different levels of theory. With this in mind, we have combined the capabilities of two open-source academic software, SHARC (Surface Hopping including Arbitrary Couplings) [1] and COBRAMM (Optimised in Bologna to Run hybrid Ab-initio and Molecular Mechanics calculations) [2], to offer an approach to perform TSH simulation within a QM/MM framework while including any arbitrary coupling [3]. Currently, the chromophore can be treated at CASSCF, ADC or TD-DFT levels of theory while the surrounding is treated classically, thanks to the already existing interfaces with third-part software. In this talk, I will first present the basic features of the interface; then I will focus on key steps for running QM/MM-TSH simulations, from the generation of the initial conditions until how to deal with MM atoms in a TSH simulation. Finally, as an exemplary application, the intersystem crossing-driven relaxation of acrolein in acetonitrile will be shown [3].



### References:

- [1] S. Mai et al: “*Nonadiabatic Dynamics: The SHARC Approach*” WIREs Comput. Mol. Sci., 8, e1370 (2018). Code available at: [sharc-md.org](http://sharc-md.org)
- [2] O. Weingart et al. “*COBRAMM 2.0 -- A software interface for tailoring molecular electronic structure calculations and running nanoscale (QM/MM) simulations*” *J. Mol. Model.* 24, 271 (2018). Code available at: <https://site.unibo.it/cobramm/en>
- [3] D. Avagliano et al. “*QM/MM Nonadiabatic Dynamics: the SHARC/COBRAMM Approach*” *J. Chem. Theory Comput.* 2021, 17, 8, 4639–4647

## How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 28

Time: Nov 25, 2021 10:00 AM Eastern Time (US and Canada)

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