Project: Controlling Excited State MD by Surface Plasmons

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Research Goals

Organic photovoltaics hold great promise for a sustainable future, but their applicability is severely limited by a relatively short exciton diffusion length within the material. In this project, we use massively parallel computing to explore in atomic detail if we can overcome this limitation by strongly coupling the material to confined light modes, as occur for example in Fabry-Pérot optical cavities (Fig. 1)

Theory and Methodology

In the strong light-matter coupling regime, electronic excitations of material and of confined light modes hybridize into new states, called polaritons, with properties of both material and light, including the high propagation velocities of the light modes. To understand if the latter also enhance the transportation of the excitation, we performed multi-scale molecular dynamics simulations of over 1000 photoactive molecules, strongly coupled to the confined light modes of Fabry-Pérot cavity. The simulations were performed with the GROMACS and Gaussian16 programs on the **Mahti** cluster.

Results: polaritonic energy transport

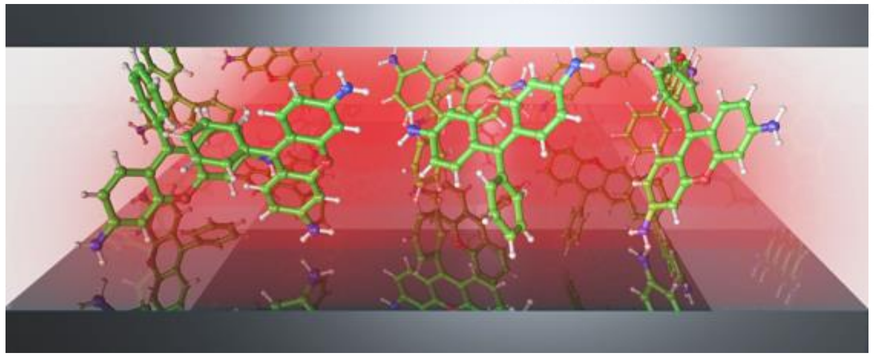

Figure 1: molecules inside Fabry-Pérot cavity

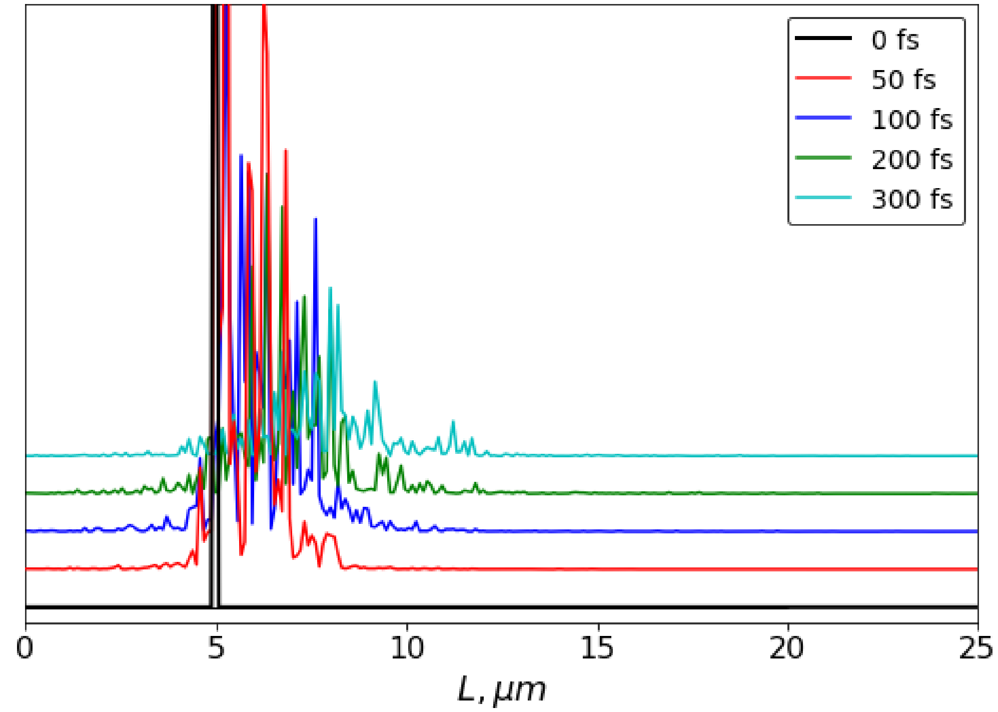

Figure 2: propagation of polaritonic wave packet

Our simulations suggest that under strong light-matter coupling exciton transport can be enhanced by orders of magnitude, reaching distances over ten micrometers.

Luk et al, *J. Chem. Theory Comput* (2017) | Groenhof et al, *J. Phys. Chem. Lett* (2019) | Tichauer et al, *J. Chem. Phys.* (2021) |