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Title: Hybrid light-matter landscapes - from single to multi-mode cavities

Abstract: It is well established that nuclei explore electronic landscapes, and that studying this exploration gives access to many key properties in chemistry and material science. Significant methodological advances have been made in the theoretical study of nuclear dynamics, from ab-initio molecular dynamics to semiclassical and nonadiabatic methods such as ring-polymer dynamics and surface-hopping.

Recently, great interest has been placed on the influence of light on materials and in particular how hybrid light-matter states develop through strong light-matter interaction. In the strong-coupling regime, light and matter become indistinguishable, and any change to the light field instantly reshapes the hybrid light-matter landscape. This has relevance to numerous fields from catalysis in chemistry to photovoltaic cells in material science and photonic qubits in quantum information science.

However, exploring hybrid light-matter landscapes is an extremely high-dimensional problem. We will therefore take advantage of the (semi)-classical methods already highly-optimised and established for nuclear dynamics. To this end, we employ the multi-trajectory Ehrenfest dynamics method, which propagates (semi)classical trajectories to ensure favorable scaling with system size. We combine it with sampling of the initial configurations from the photonic Wigner distribution at zero temperature to preserve the quantum nature of the light. By coupling the photon dynamics to real-time time-dependent density functional theory, we make the exploration of this extremely complex hybrid light-matter landscape possible, and our approach constitutes not only a novel and intriguing method development but also enables, for the first time, the investigation of quantum optics effects in real molecules.

In particular, we study quantum phenomena important to quantum computing in molecules interacting with a wave guide, which will ultimately allow us to explore materials capable of forming photonic qubits. In this talk, we will explore how the semiclassical Ehrenfest dynamics are affected when going from a single to a multimode setup for both model systems and real molecules.