Unveiling chemical reactivity using invariant manifolds
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The usual identification of reactive trajectories for the calculation of reaction rates requires very time-consuming simulations, particularly if the environment presents memory effects. In this talk, we will discuss how invariant manifolds can be used to identify reactive trajectories in a system that interacts with the environment. We will also show how invariant manifolds can be used to compute reaction rates perturbativelly, accounting for the effect of anharmonities beyond Kramer's and Grote-Hynes's theories.