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### Quantum dynamics

The quantum treatment of gas-phase chemical reaction dynamics in the Born-Oppenheimer regime requires solving the Schrödinger equation for the motion of nuclei on one or a manifold of potential energy surfaces (PESs) associated with the electronic states of a molecular system. The solution of the nuclei Schrödinger equation, which can be cast either in a time-dependent (TD) or a time-independent (TI) form, is then matched to proper asymptotic conditions to get the elements of the so-called scattering matrix, corresponding to the quantum mechanical reaction probability amplitude, out of which observable properties can be extracted to be compared with the outcome of crossed-molecular-beam experiments.

Ideally, accurate values of the electronic energies should be promptly available at all geometries needed by the dynamics calculations. This is commonly and efficiently achieved by adopting analytic functional representations of the PES, which fit or interpolate a set of energies computed at a number of geometries by high-level ab initio methods.

In this lecture, all above outlined aspects will be covered with a focus on performing quantum dynamics calculations on distributed architectures. Accordingly, methods for 1) selecting the most suitable set of geometries 2) performing electronic-structure calculations 3) fitting/interpolating the obtained set of energies 4) running the dynamics will be reviewed and organized in a workflow which will be the subject of the hands-on session. Applications of interest in astrochemistry will also be shortly illustrated.