

Motivation: PES-to-RateCoeff Approach



Collision Generating an Exchange Reaction:





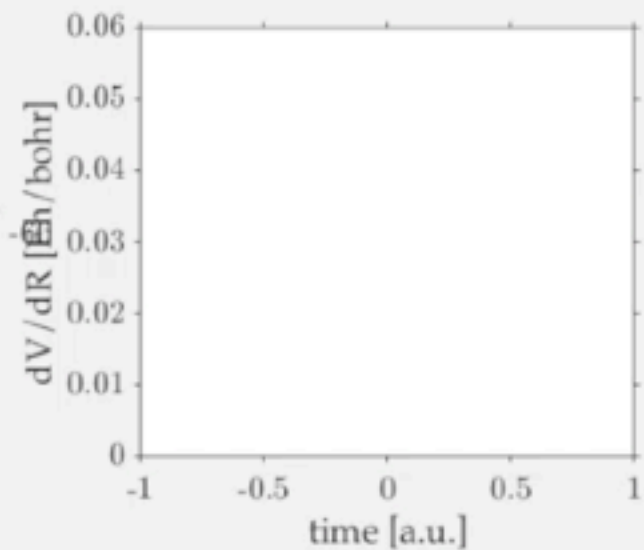
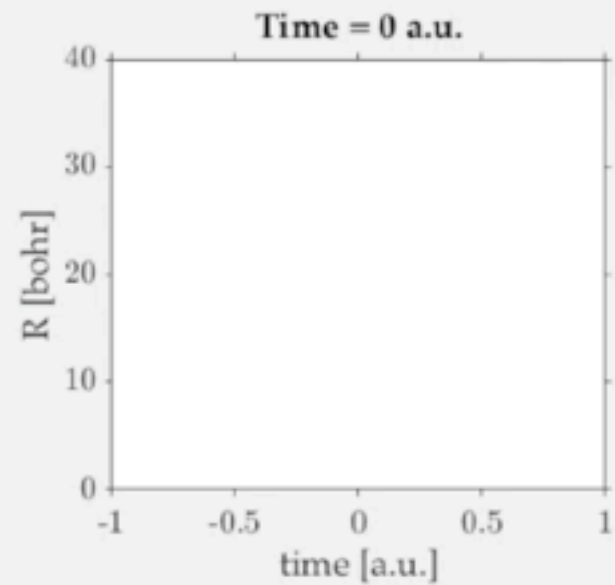
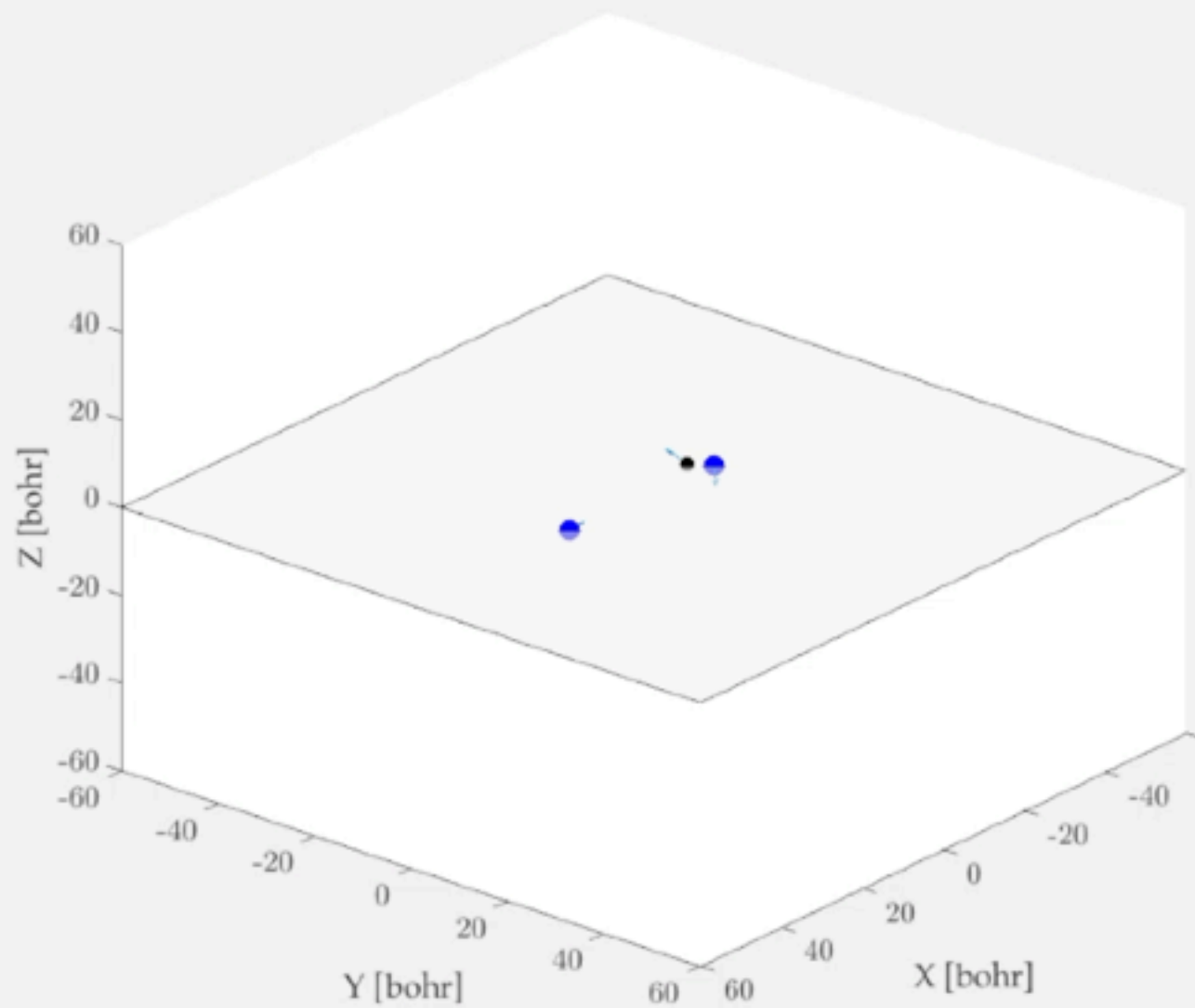
QCT

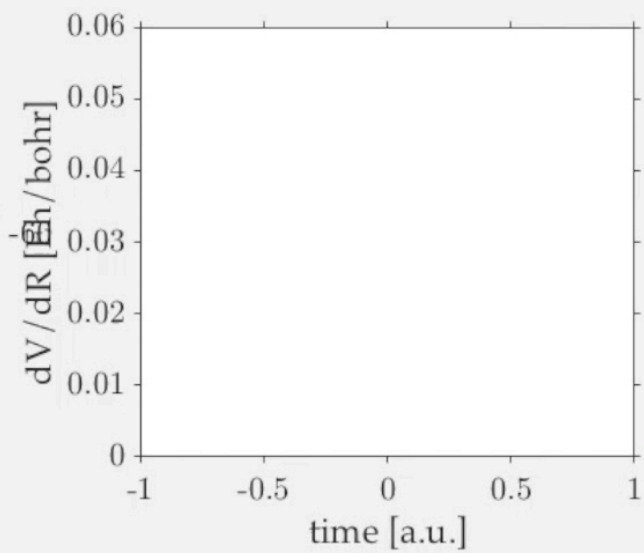
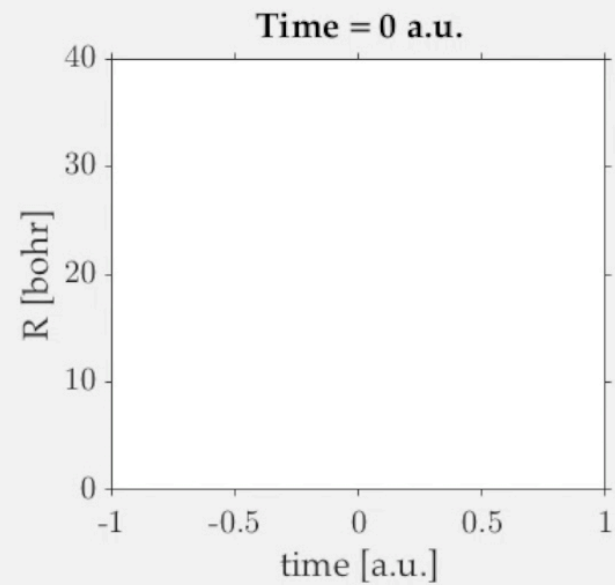
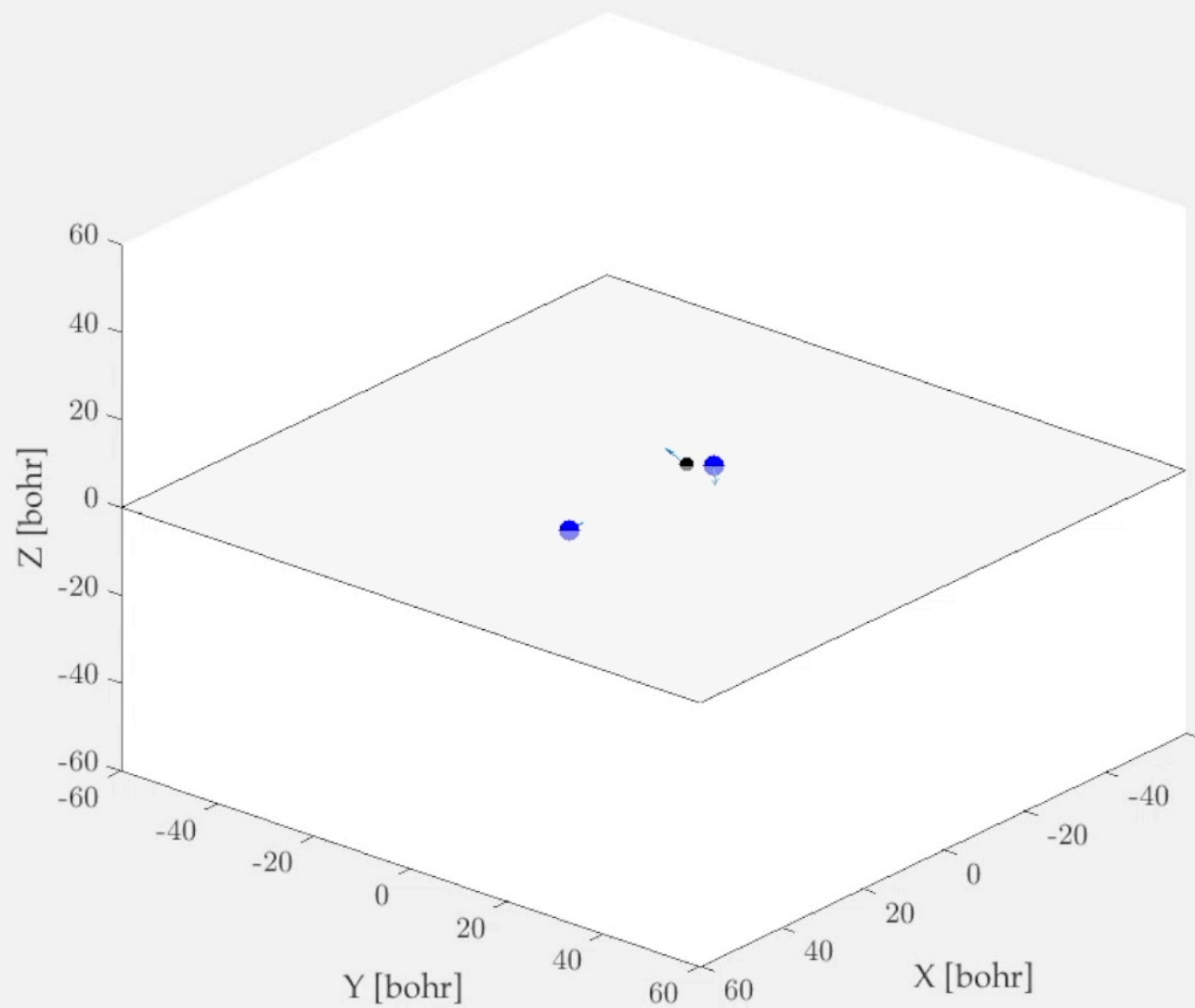
PES



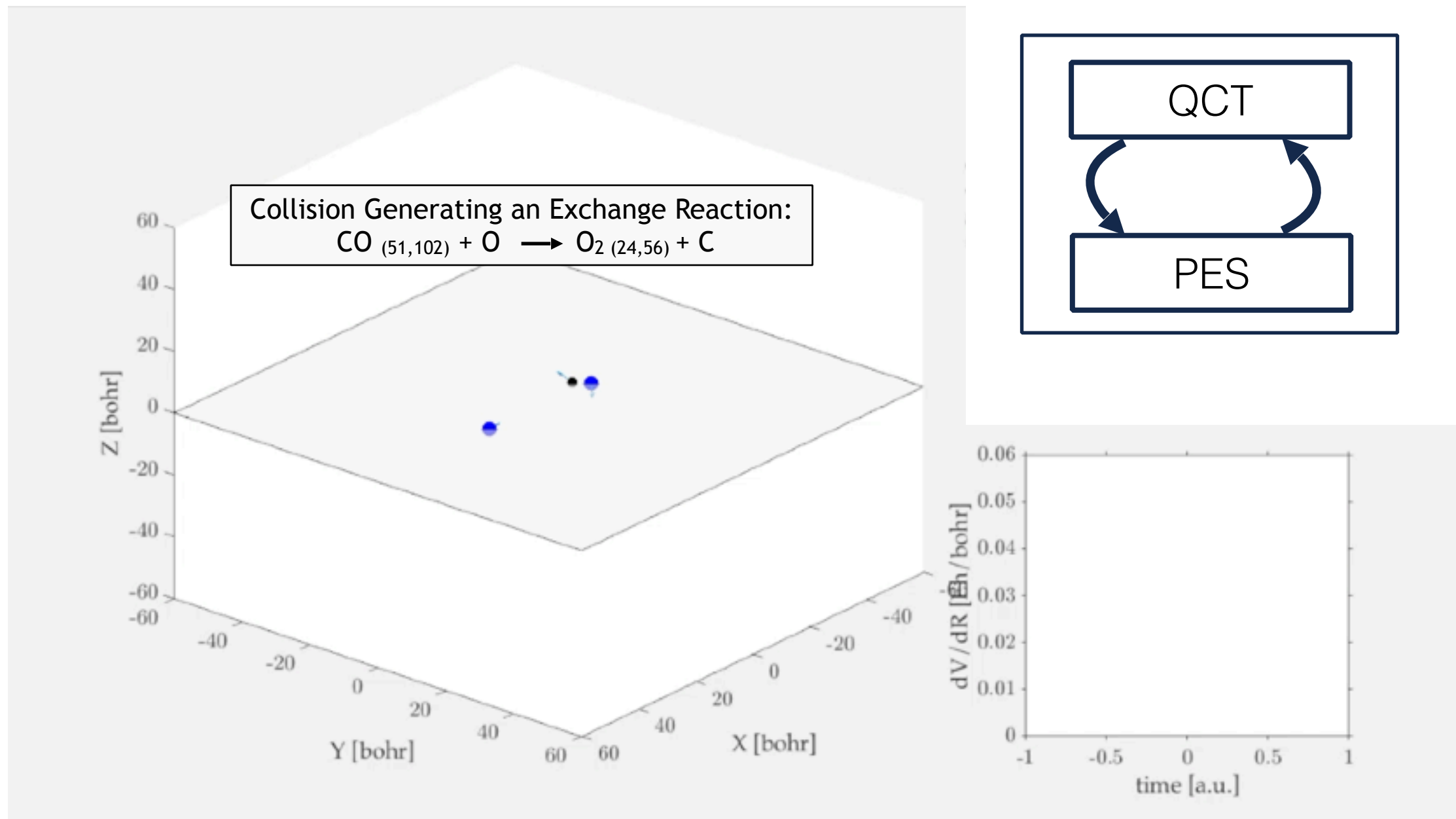


1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as source terms of the Hamiltonian Eq.s for the calculation of atom trajectories;



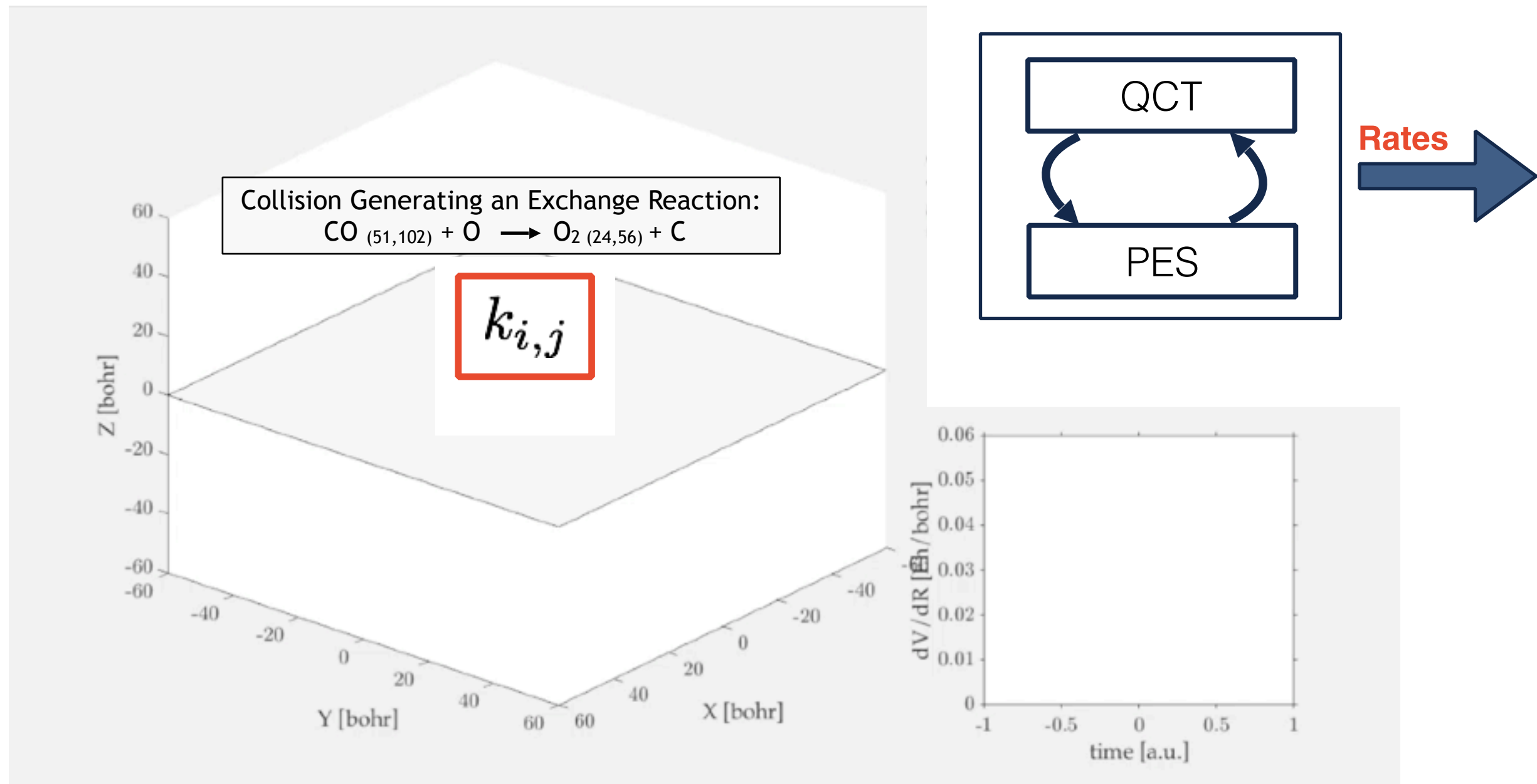


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1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as **source terms of the Hamiltonian Eq.s** for the calculation of atom trajectories;
2. Rate Coefficients are finally obtained **by integrating** over Maxwellian distributions of collisional energies.

PESs drive the collision dynamics, and govern the values of rate coefficients