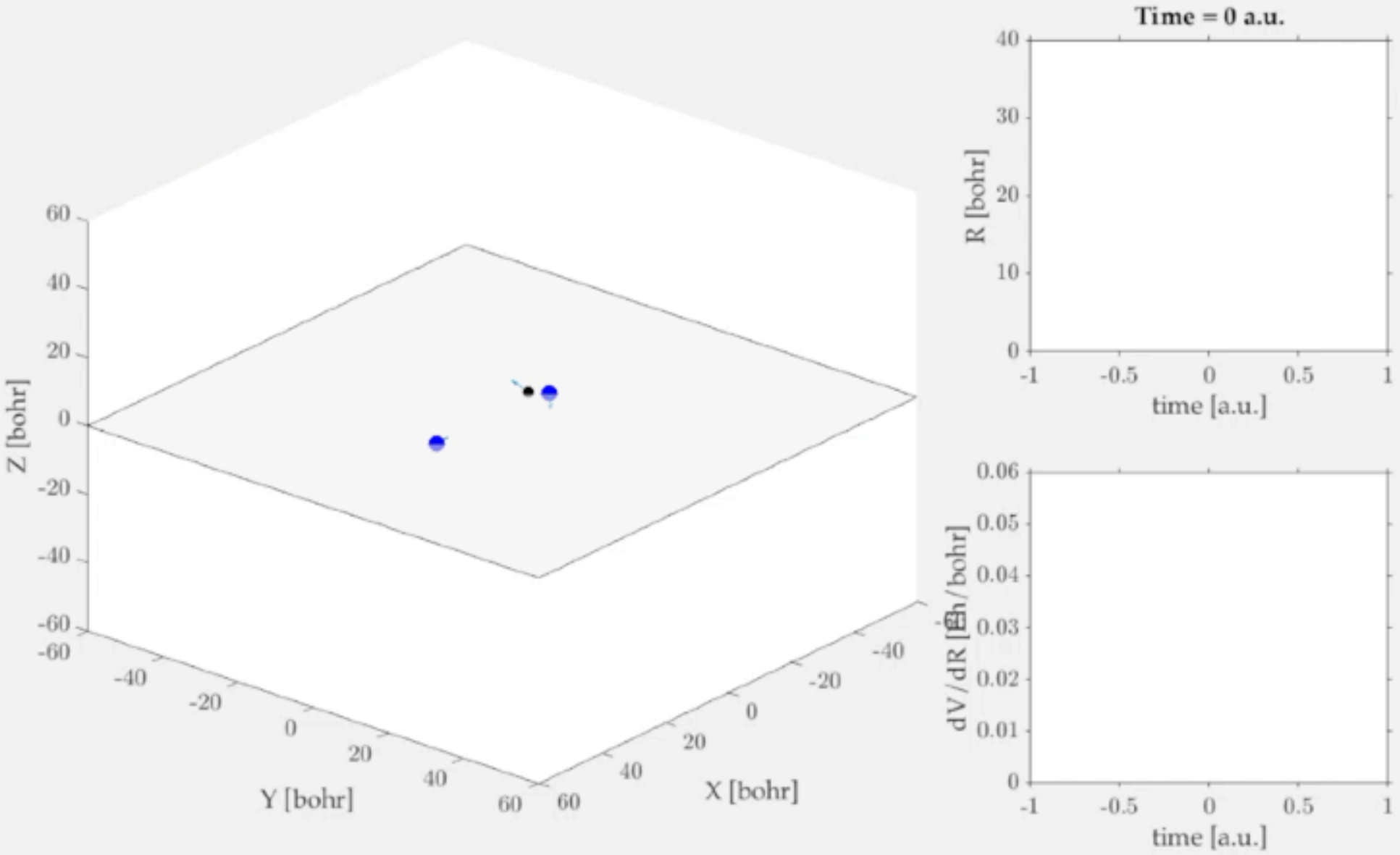

Time = 0 a.u.
R [bohr]
time [a.u.]
dV/dR [Eh/bohr]
time [a.u.]
Z [bohr]
Y [bohr]
X [bohr]

Motivation: PES-to-Rate Coeff.s Approach

9

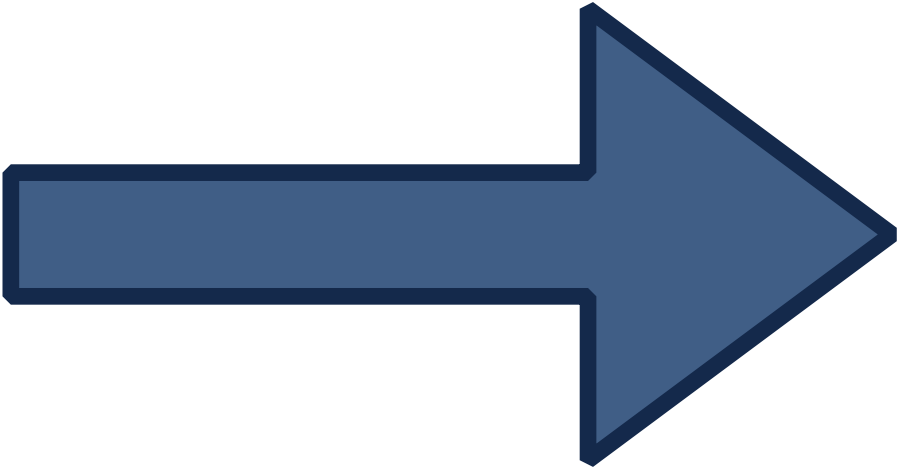
1. Cross Sections are computed by means of QCT, in which the **gradients of the Potential Energy Surface (PES)** are considered as **source terms of the Hamiltonian Eq.s** for the calculation of atom trajectories;

2. Rate Coefficients are finally obtained **by integrating over Maxwellian distributions** of collisional energies.

Collision Generating an Exchange Reaction:

$$CO_{(51,102)} + O \longrightarrow O_{2\,(24,56)} + C$$

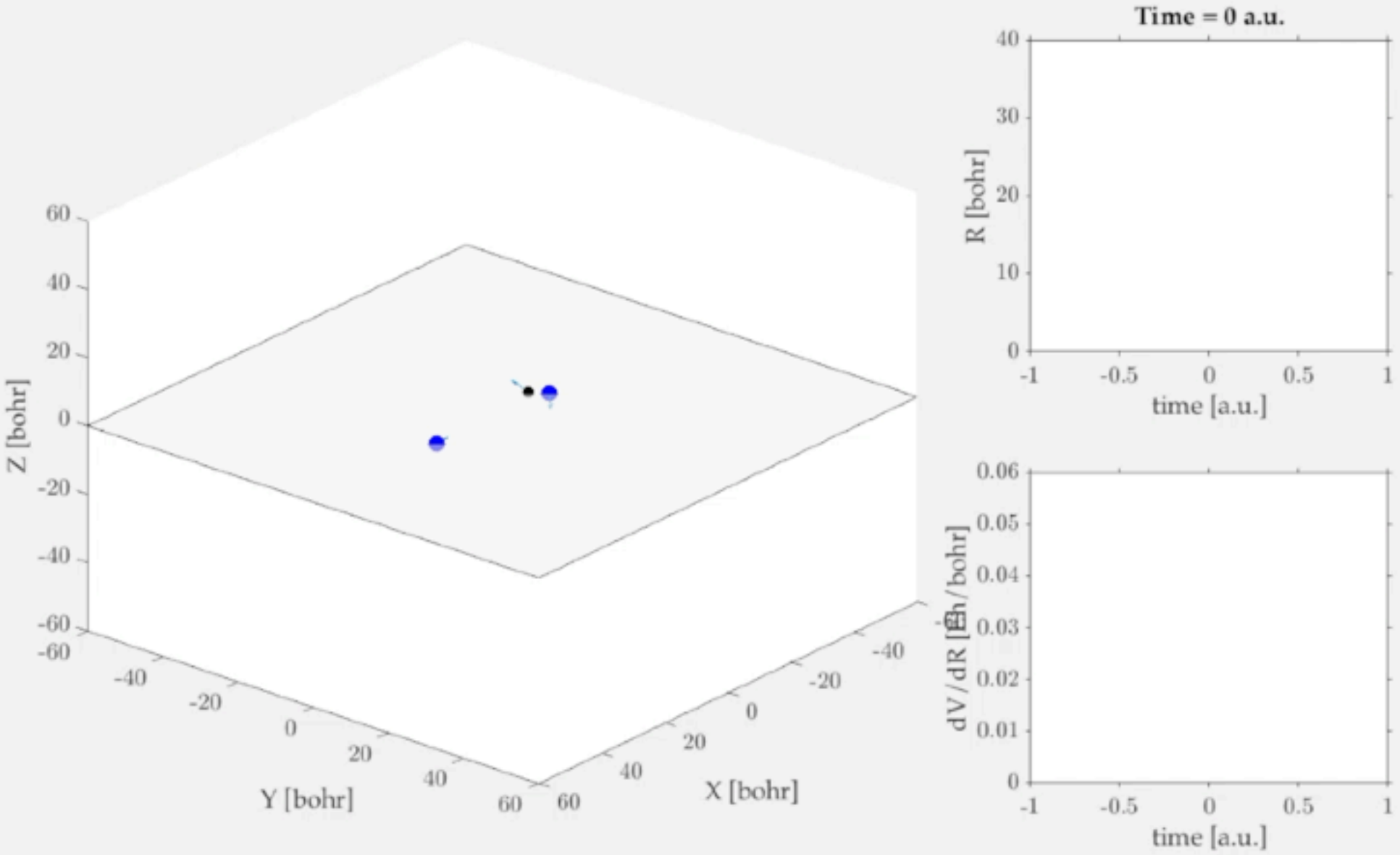
PESs drive the collision dynamics, and govern the values of rate coefficients



QCT

PES

Rates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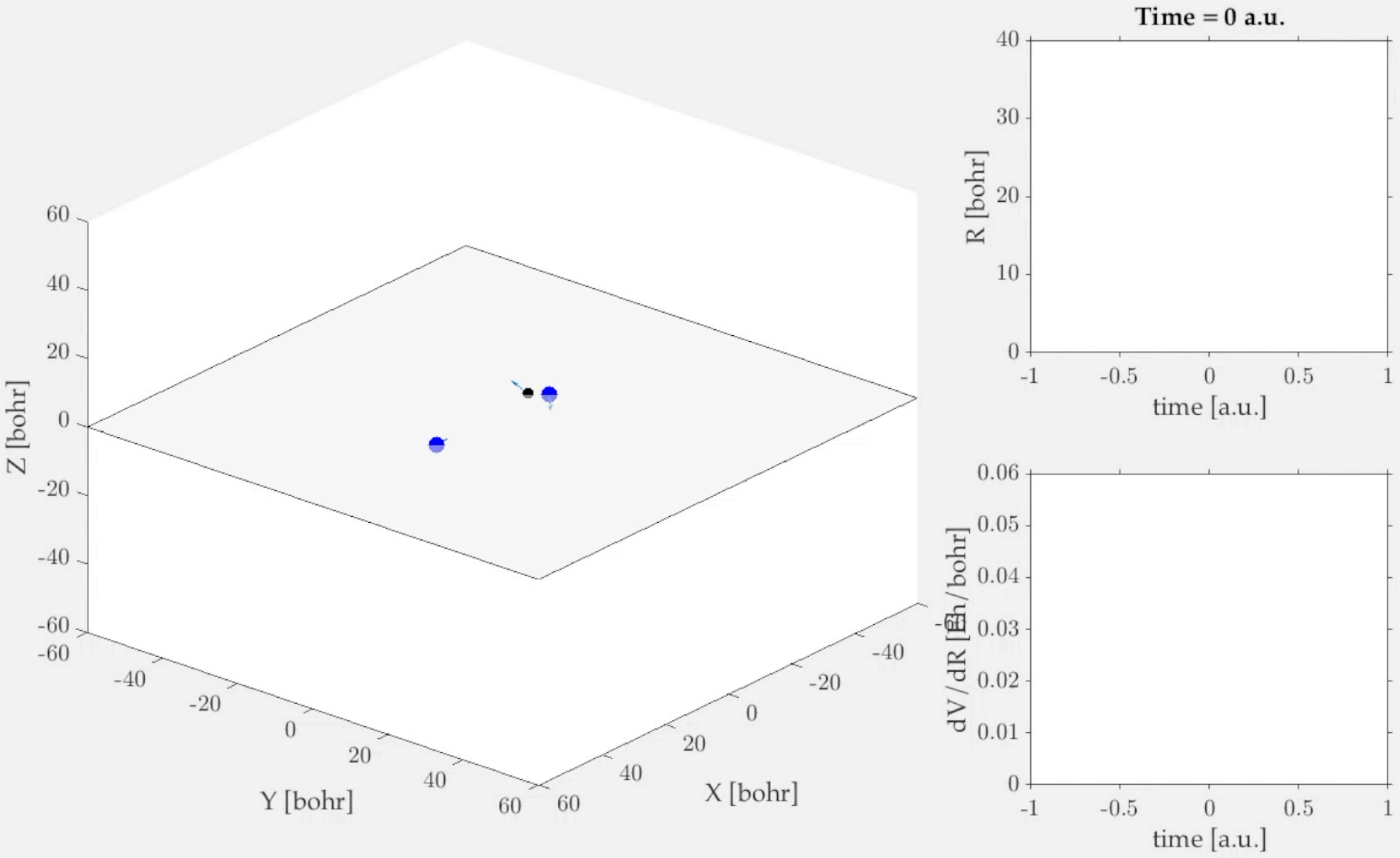
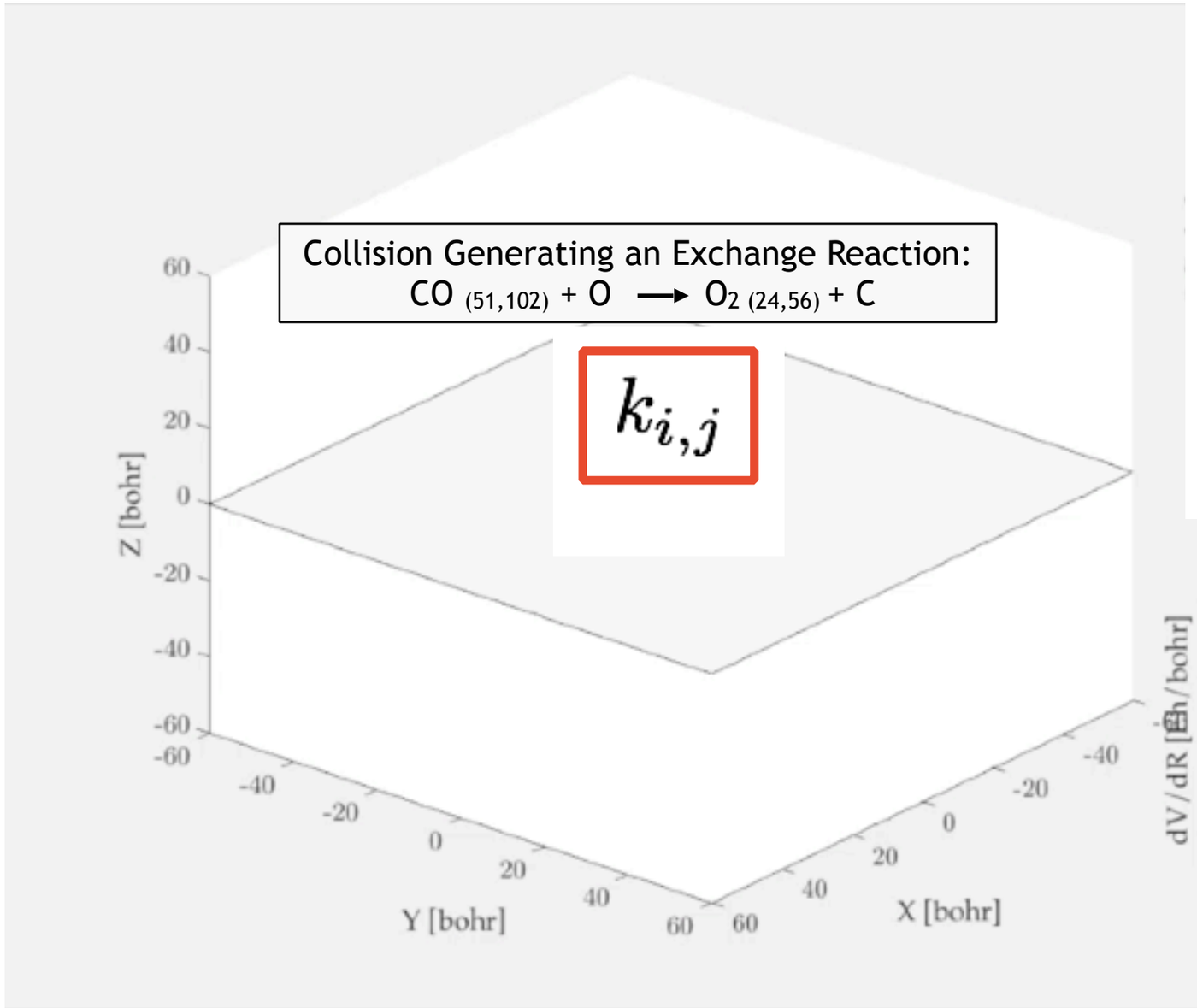
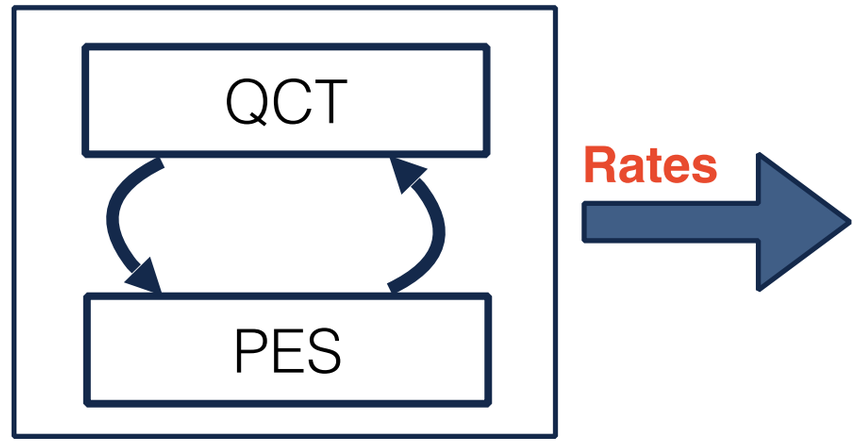
R [bohr]
time [a.u.]
dV/dR [Eh/bohr]
time [a.u.]
Z [bohr]
Y [bohr]
X [bohr]


Time = 0 a.u.
R [bohr]
time [a.u.]
dV/dR [Eh/bohr]
time [a.u.]
Z [bohr]
Y [bohr]
X [bohr]

Motivation: PES-to-Rate Coeff.s Approach





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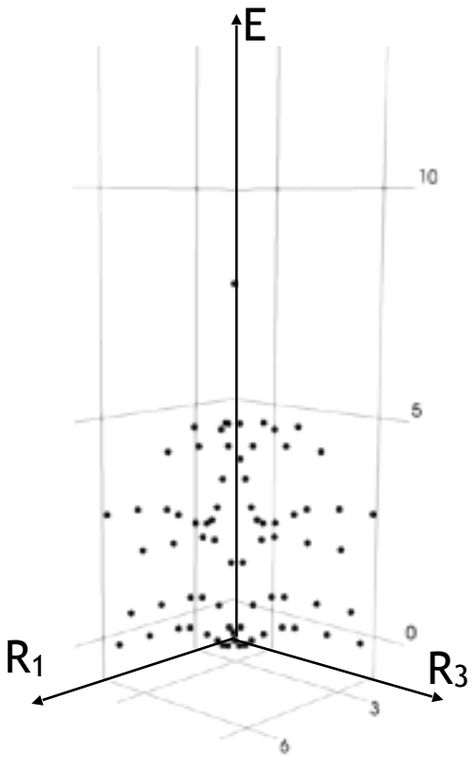
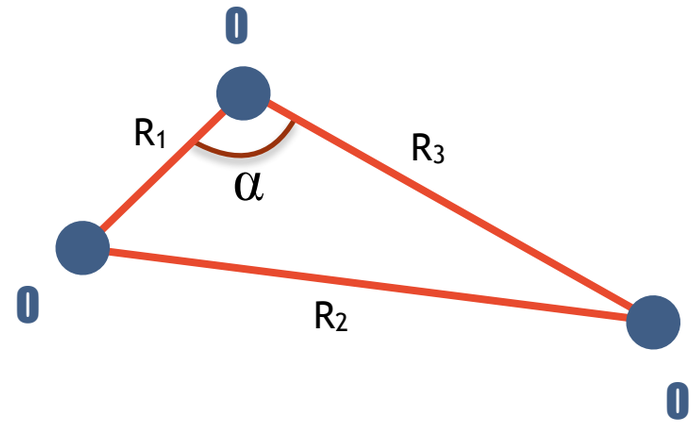
PESs drive the collision dynamics, and govern the values of rate coefficients

Motivation: PES

Potential Energy Surfaces (PESs) are functions that describe the **quantum-physics interactions between atoms.**





Ab-Initio PES Generation Process:

1. A large number of atom **geometric arrangements** (R_1,R_2,R_3) is selected;
2. **Electronic Schrödinger Eq.** is solved at such arrangements;
3. The resulting energies are **fit to analytical expressions**.