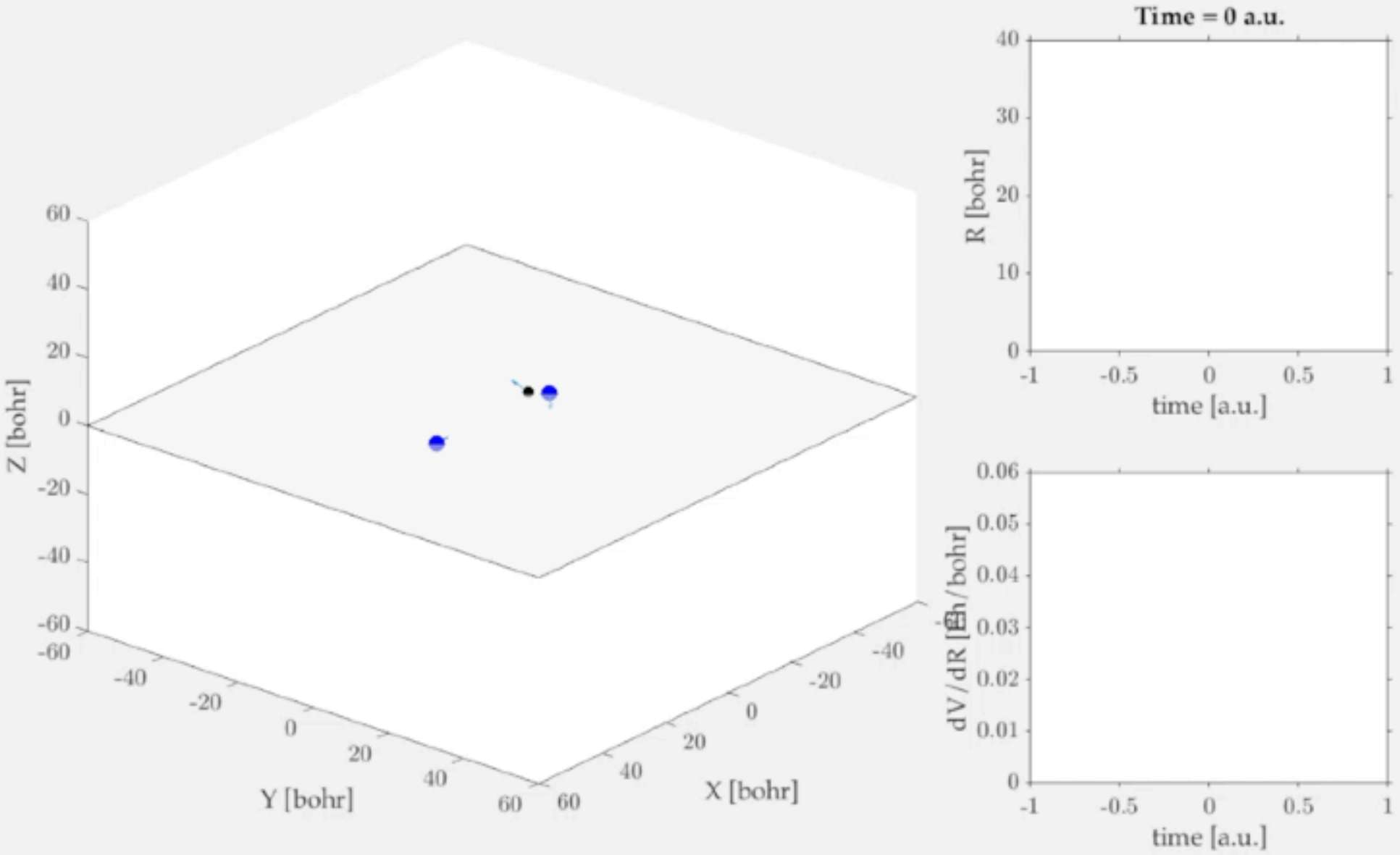

Time = 0 a.u.
R [bohr]
time [a.u.]
dV/dR [Eh/bohr]
time [a.u.]
Z [bohr]
Y [bohr]
X [bohr]

Motivation: PES-to-Rate Coeff.s Approach

9

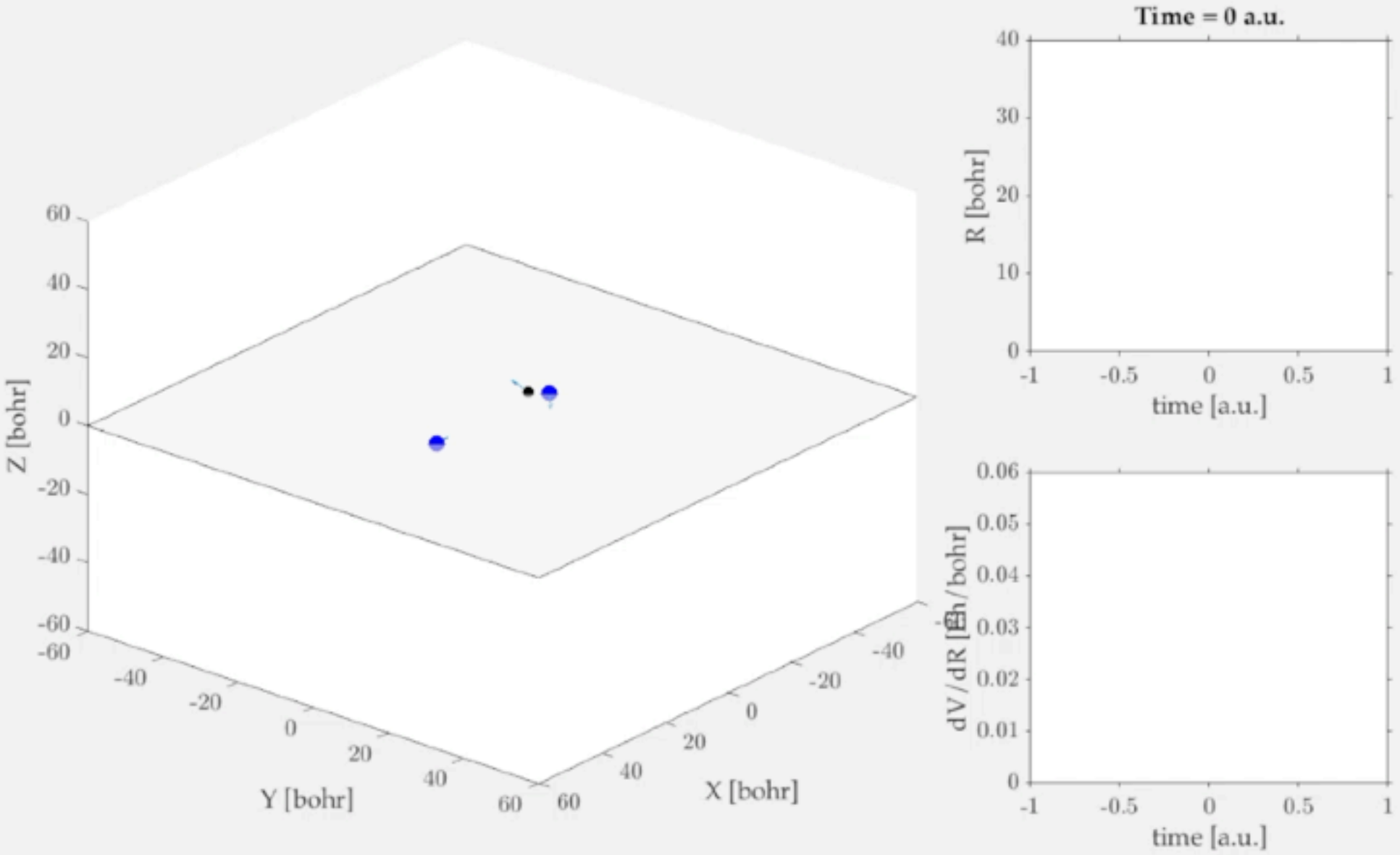
Collision Generating an Exchange Reaction:

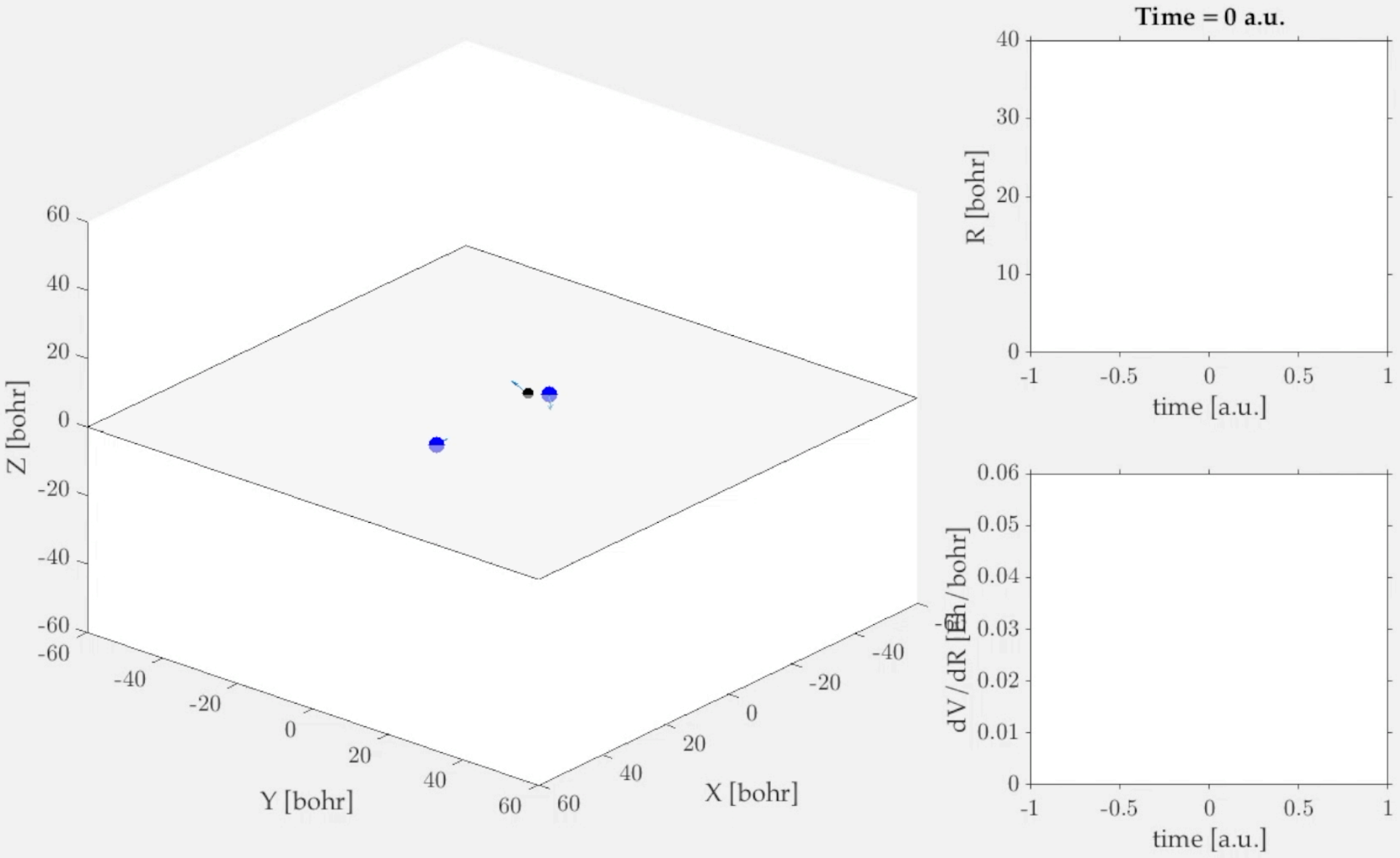
$$CO_{(51,102)} + O \longrightarrow O_{2\,(24,56)} + C$$

QCT

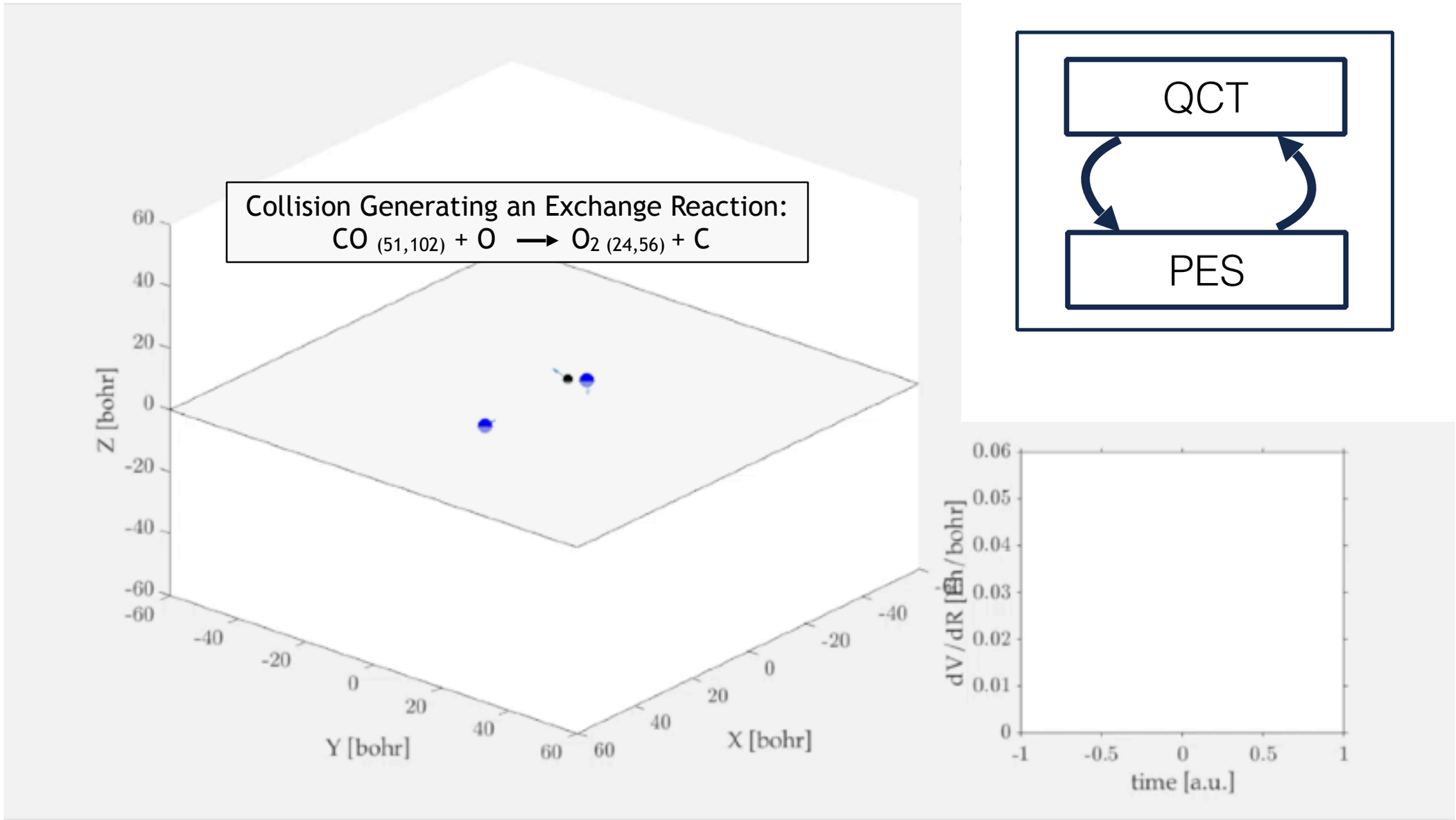
PES

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;


Time = 0 a.u.
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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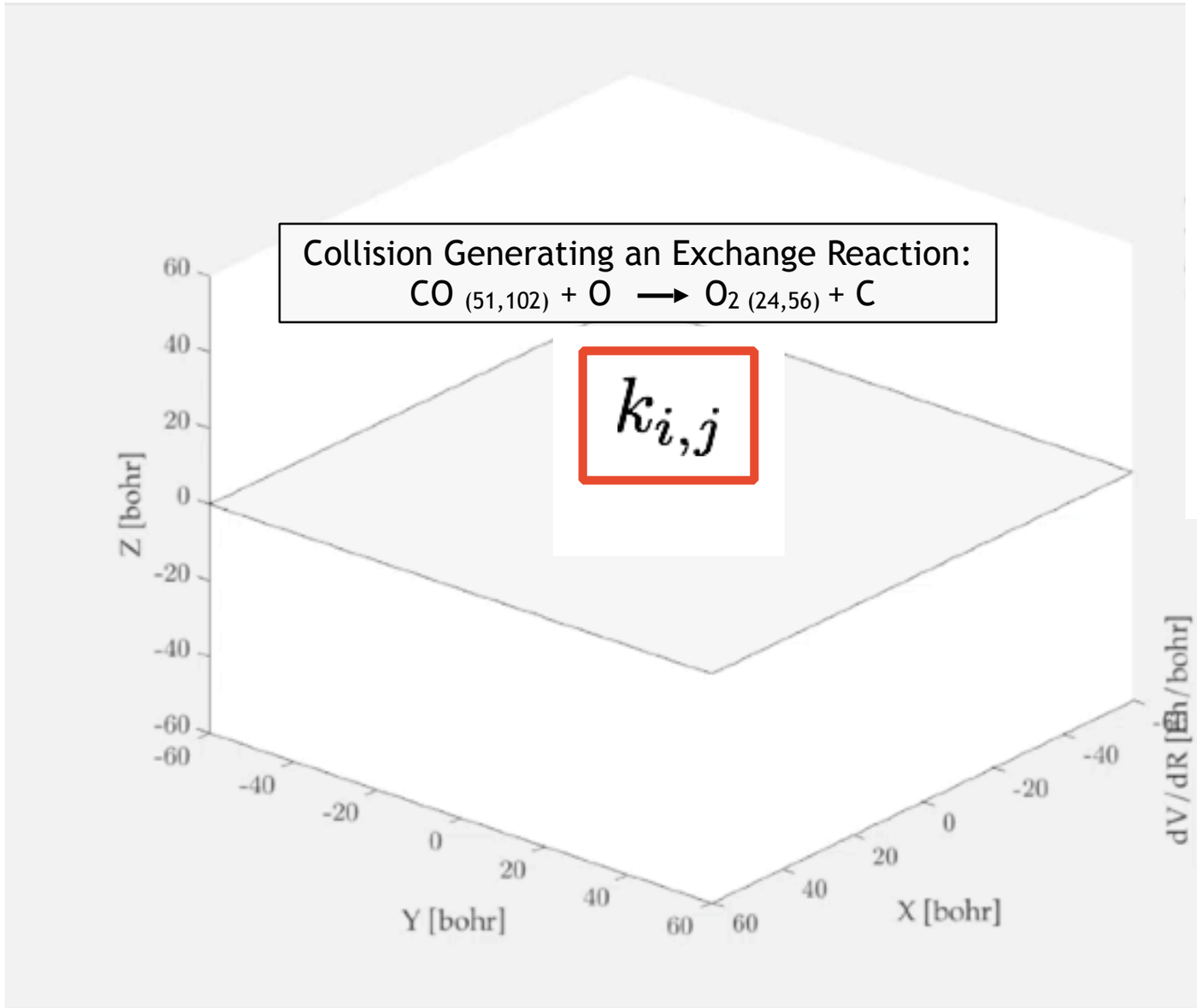
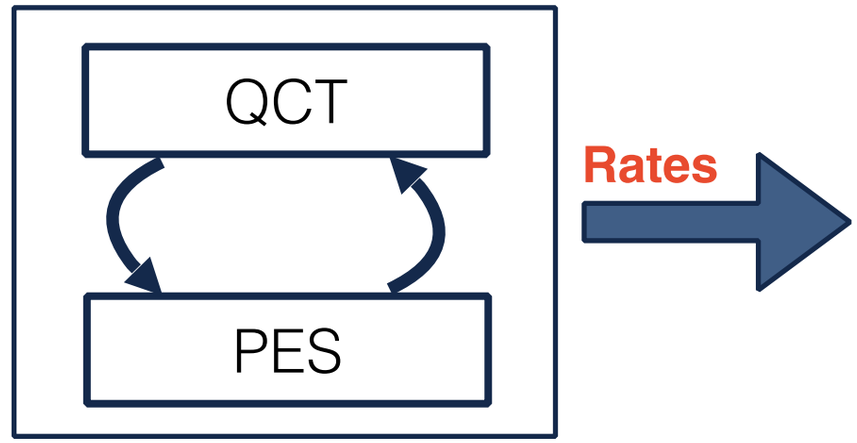
Motivation: PES-to-Rate Coeff.s Approach





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