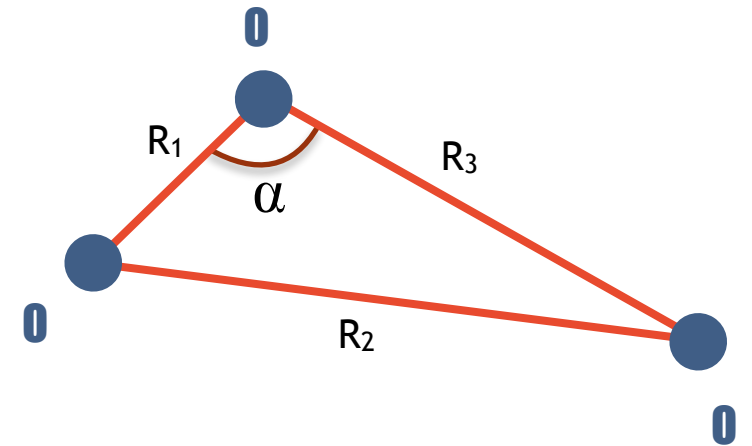
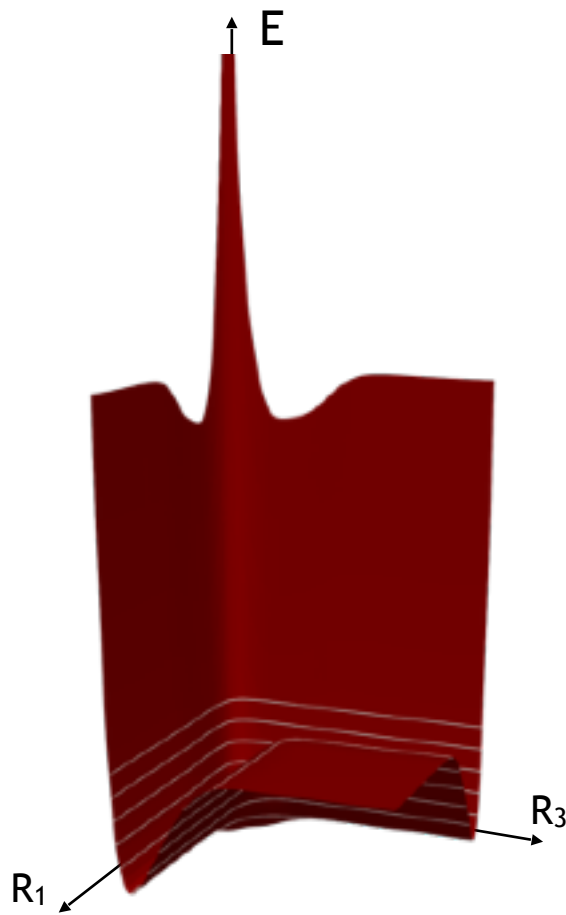


Motivation: PES

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**.

Each research group typically has its distinctive protocols to PES generations.

The result is that the surfaces for a given collisional system are diverse from one laboratory to the other.

- The process is extremely time consuming;
- There is no systematic approach in place in order to evaluate the “cost” of such differences.

Motivation: Effects of PES Uncertainty

$$\begin{cases} \frac{d\mathbf{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{q}} \\ \frac{d\mathbf{q}}{dt} = +\frac{\partial \mathcal{H}}{\partial \mathbf{p}} \end{cases} \quad \mathcal{H} = T + V$$

