# ML for PESs: Introduction

In the last decade there has been an increasing effort in taking advantage of Machine Learning for constructing Potential Energy Surfaces. In particular, using:

- ✦ **Gaussian Processes**

- ✦ **Neural Network**

- ✦ *"Representing Global Reactive Potential Energy Surfaces Using Gaussian Processes"*, *J. Phys. Chem. A 2017*;
- ✦ "Comparison of permutationally invariant polynomials, neural networks, and Gaussianapproximation potentials in representingwater interactions through many-bodyexpansions", J. Chem. Phys. 2018;
- ✦ "Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces", Phys. Rev. Lett. 2007;
- ✦ "Permutation invariant potential energy surfaces for polyatomic reactions using atomistic neural networks", J. Chem. Phys. 2016;
- ✦ …

However, almost the entire literature focuses on the relatively low energy part of the PES.

> **Through this work, we want to assess if the ML reconstruction can achieve reasonable accuracy for the region of the surface of Hypersonic interest.**
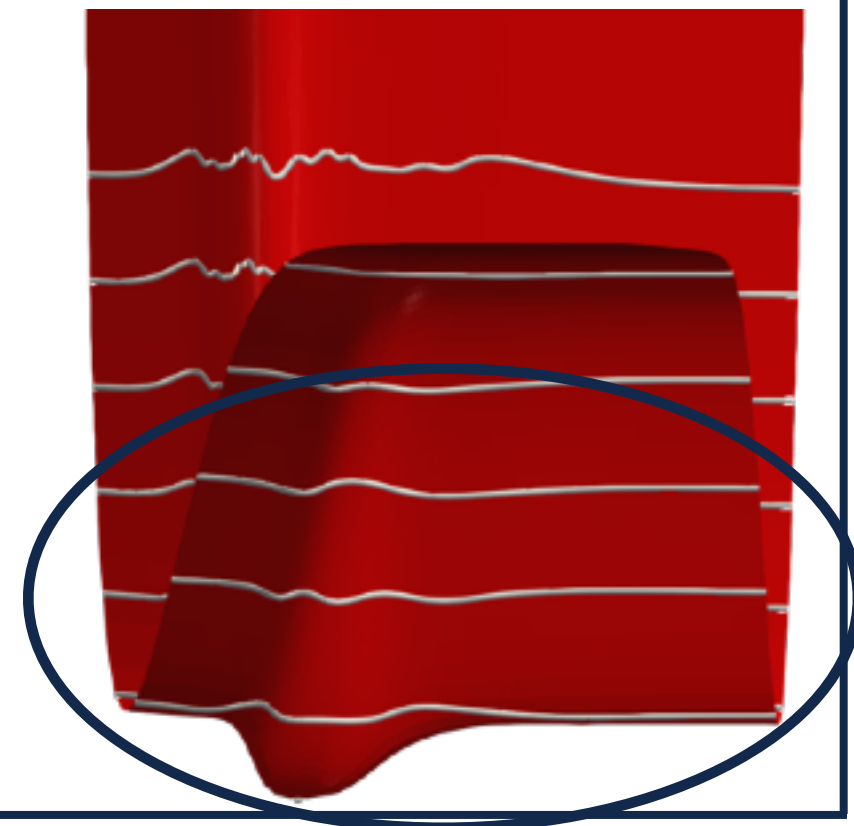
ANN for PESs: Methodology

Multi-layer feed-forward Neural Networks (NN) have been adopted **as fitting functional**:

- ✦ Easy to implement;
- ✦ Easy to train;
- ✦ Easy to generalize to new systems;
- ✦ Easy to differentiate in **R**;

- ✦ Cost effective;
- ✦ Easy to be refined;
- ✦ Widely tested;
- ✦ Easy to be extended to the stochastic case.

Permutation Invariant Polynomials Neural Networks (PIP-NN):

theano

Lasagne

1. A **Symmetrized Polynomial Vector** (**G**) is constructed, in order to account for the permutation symmetries; for example, for a A3-type system:

$$G_1 = p_1 + p_2 + p_3$$
$$G_2 = p_1 p_2 + p_2 p_3 + p_1 p_3$$
$$G_3 = p_1 p_2 p_3$$

where $p_i = \exp(-\lambda_i(R_i - r_{e_i}))$, being λ_i and r_{e_i} tunable parameters.

R_1

R_2

R_3

⋮

R_N