**Introduction**

In the electrochemistry course you learned about an important quantity, the exchange current, and how it reflects how viable is the reaction kinetics of an electrochemical transformation.

In this experiment you will predict what is the most efficient metal catalyst for hydrogen evolution by plotting the adsorption energy for hydrogen on different metals versus the measured exchange currents for this reaction. According to the Sabatier principle (named after the chemist Paul Sabatier), high catalytic activity is associated to an interaction between reactants and catalysts, which needs to be neither too strong nor too weak. As a consequence, the plot will have a maximum corresponding to the to the most active catalyst and the ideal adsorption energy: you will observe a so-named volcano plot.

You will learn how to:

* Evaluate the chemisorption energy for an atomic species on a metal;
* generate a volcano plot describing trends in catalytic activity for Hydrogen evolution;
* use the most basic feature of Unix operating system and work remotely on our hpc cluster login.hpc.ic.ac.uk;
* use a quantum-mechanical programme, CP2K, which implements Density Functional Theory (DFT), to calculate the adsorption energies for Hydrogen on the closely packed surfaces of different metals;
* control and evaluate
  + the numerical error in your DFT calculations
  + the error associated to the selection of simulation parameters such as set of k points used to sample the Brillouin zone and the basis set used to expand the orbitals. Predict the equilibrium lattice parameters for a metal;
* extract from these calculations optimised geometries and energies, and evaluate adsorption energies;
* use a visualization programme to represent relaxation trajectories and optimised configurations.

Pt-H ENERGY| Total FORCE\_EVAL ( QS ) energy (a.u.): -7687.745893106200128

Mo-H ENERGY| Total FORCE\_EVAL ( QS ) energy (a.u.): -4366.408591960806916

Au-H ENERGY| Total FORCE\_EVAL ( QS ) energy (a.u.): -2128.098453575051735

Ag-H ENERGY| Total FORCE\_EVAL ( QS ) energy (a.u.): -2369.830342421368641

H2 ENERGY| Total FORCE\_EVAL ( QS ) energy (a.u.): -1.164851668533423