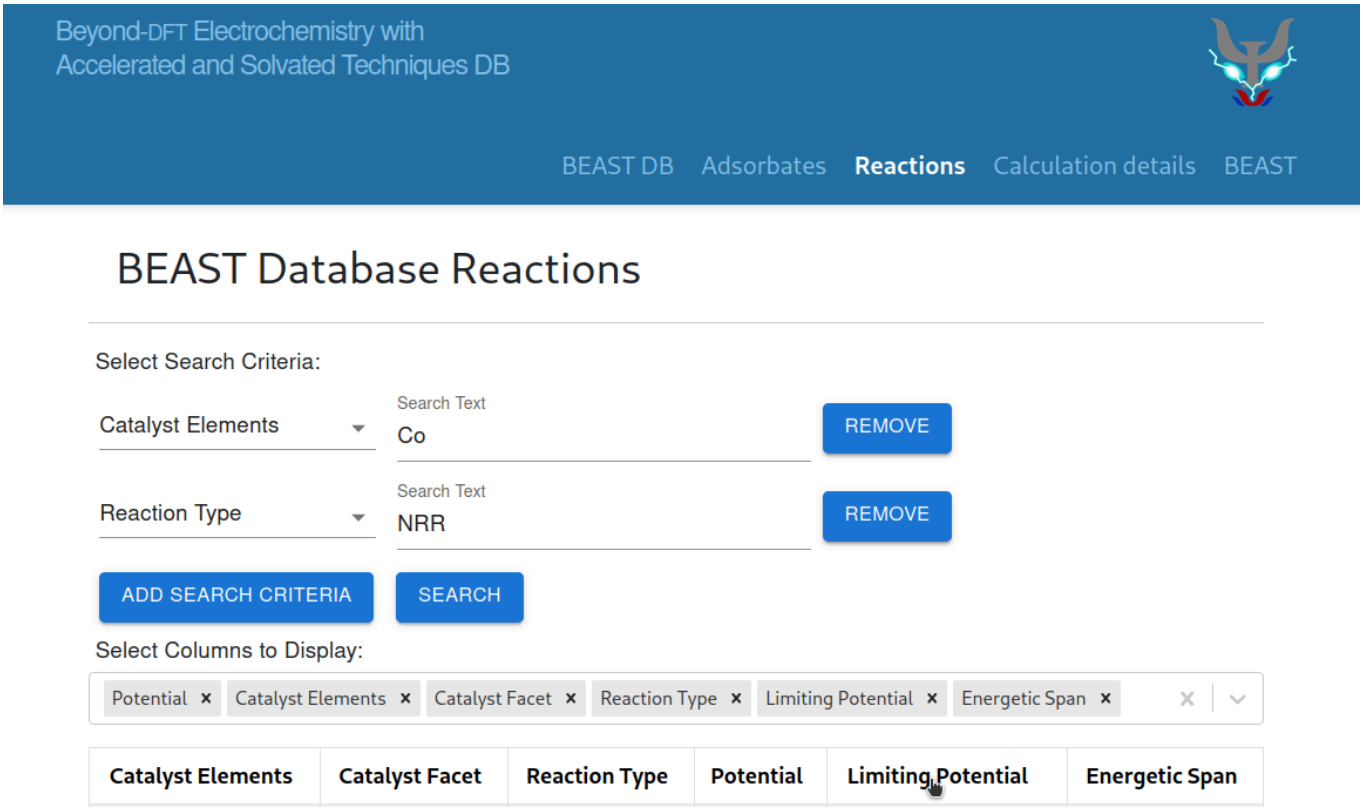
BEAST DB Tutorial

Reactions for Metal Surfaces

Let's start with a metal surface calculation. Navigate to the reaction search page, and create a search with catalyst elements: Co and reaction type: NRR for nitrogen reduction reaction.



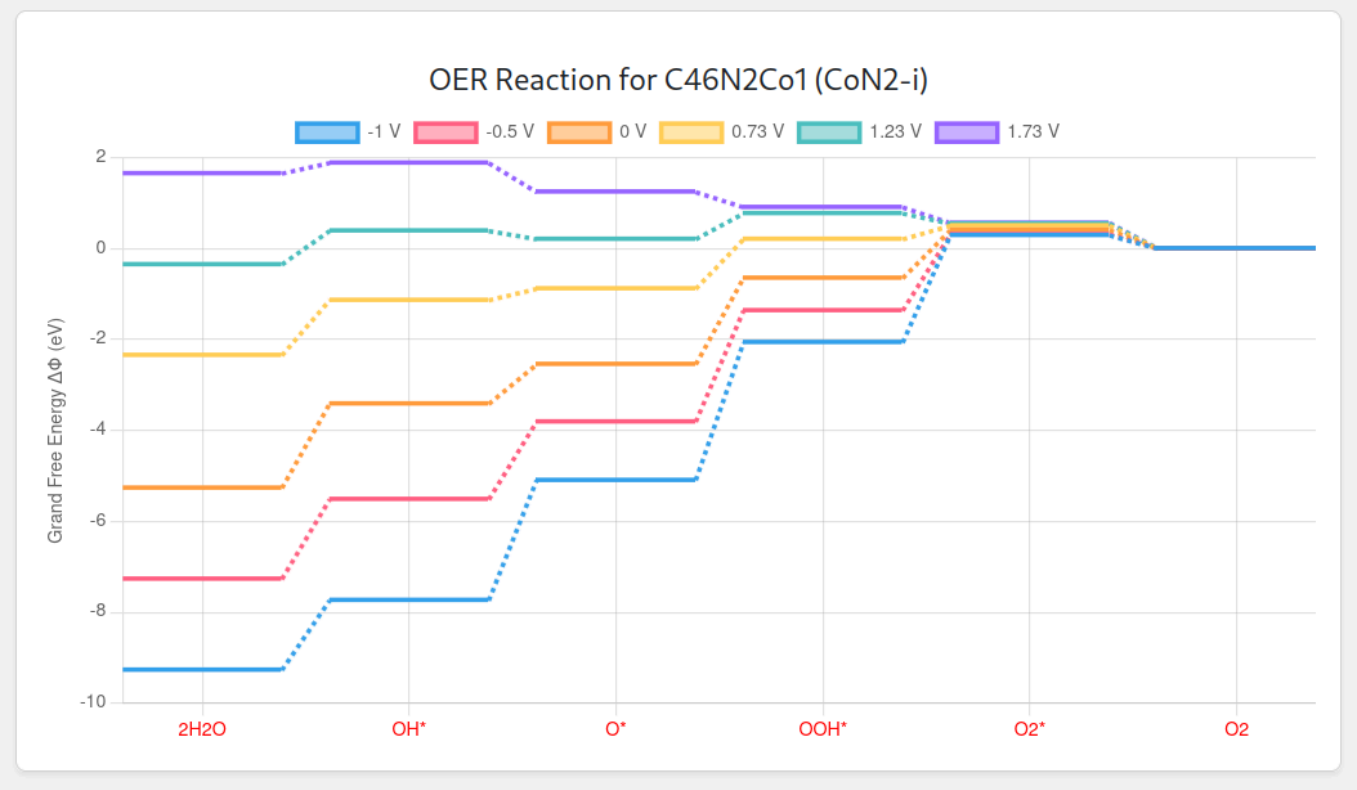
Click on the "Limiting potential" column header twice to sort by the limiting potential in ascending order. The very first row will now show the reaction with the smallest limiting potential. Click on it to navigate to the reaction view.

The reaction view will show a graph plotting each of the steps in this reaction. Click on one of the lines corresponding to the NNH2* reaction to navigate to the adsorbed state page for this calculation.

This page shows a 3D view of the final structure for this calculation and a plot of adsorption energy versus applied potential. Click on one of the points at a different active site (in yellow) at to view the corresponding state page. Consider why the calculation with the highest adsorption energy at -0.5 V might be less stable.

Reactions for MNC Systems

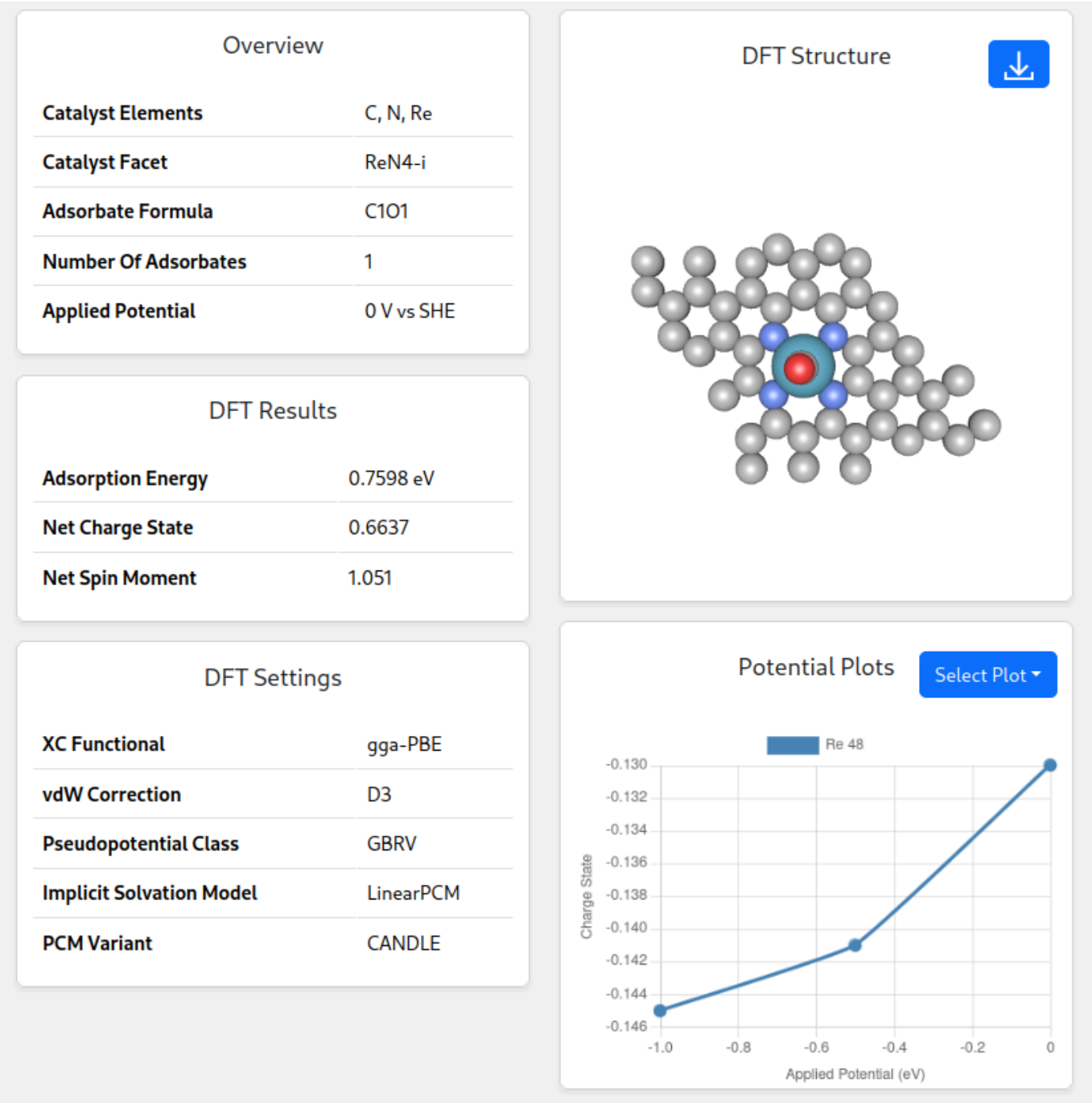
This database contains a significant amount of reactions on MNC surfaces.
Navigate to the reaction search page and create a search with catalyst elements:
"C Co" and reaction type "OER" for oxygen evolution reaction.



Click on the reaction for the CoN2-i facet, and identify the most endothermic step at 1.23 V applied potential. Find the corresponding system replacing Co
with Fe, and identify the rate limiting step for this system at this potential. Compare these and suggest why they may be different.

Adsorbed States

Navigate to the adsorbed state page, and create a search for catalyst elements:
"C Re", adsorbate formula "C1O1", and catalyst facet "ReN4-i". Click on the zero volt calculation to open the adsorbed state page.



On this page, view the charge on the C and O atoms and note their charge states. Let's compare CO adsorption on a different MNC catalyst to see if the charges change with the binding energy. Find the ZrN4-i catalyst at 0 V and compare the same charge states and adsorption energy. In our referencing scheme, the adsorption energy is actually the desorption process, so a highly positive value implies favorable binding. Based on the charges, can you rationalize the significantly more favorable binding of CO on Zr?