# Deloitte's Quantum Climate Challenge 2023

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## 1 Introduction

The code in the following github
*https* : *//github.com/jsaroni/vqe_co2_global_warming_active_space*
gives a vqe algorithm for finding the ground state as described in the detailed description of the quantum climate challenge for different compounds and metals. Different approaches can be used in the code and I would be happy to include them. These involve using a adaptive approaches, entanglement forging from circuit knitting, orbital freezing, and running on a real quantum computer with error mitigation. By varying the bond length from the metal, one can general potential energy curves and compare to the following curves from quantistry. Given a large collection of the same metal organic framework, each of which is independent of all others, the total potential energy would scale linearly with their number.

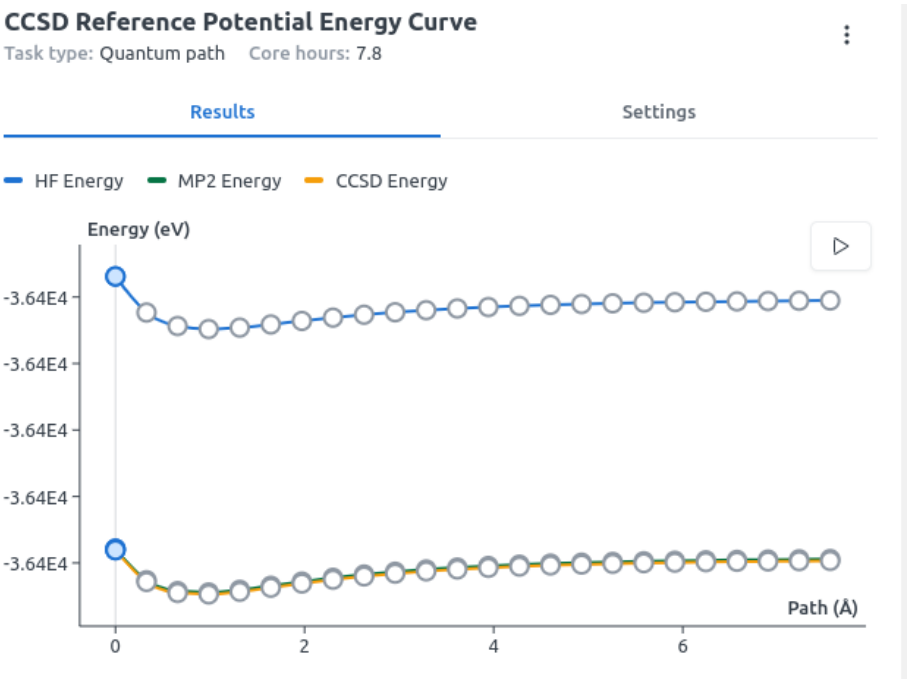
CCSD Reference Potential Energy Curve
Task type: Quantum path
Core hours: 7.8
Results
Settings
HF Energy
MP2 Energy
CCSD Energy
Energy (eV)
-3.64E4
-3.64E4
-3.64E4
-3.64E4
-3.64E4
Path (Å)
0
2
4
6

Figure 1:

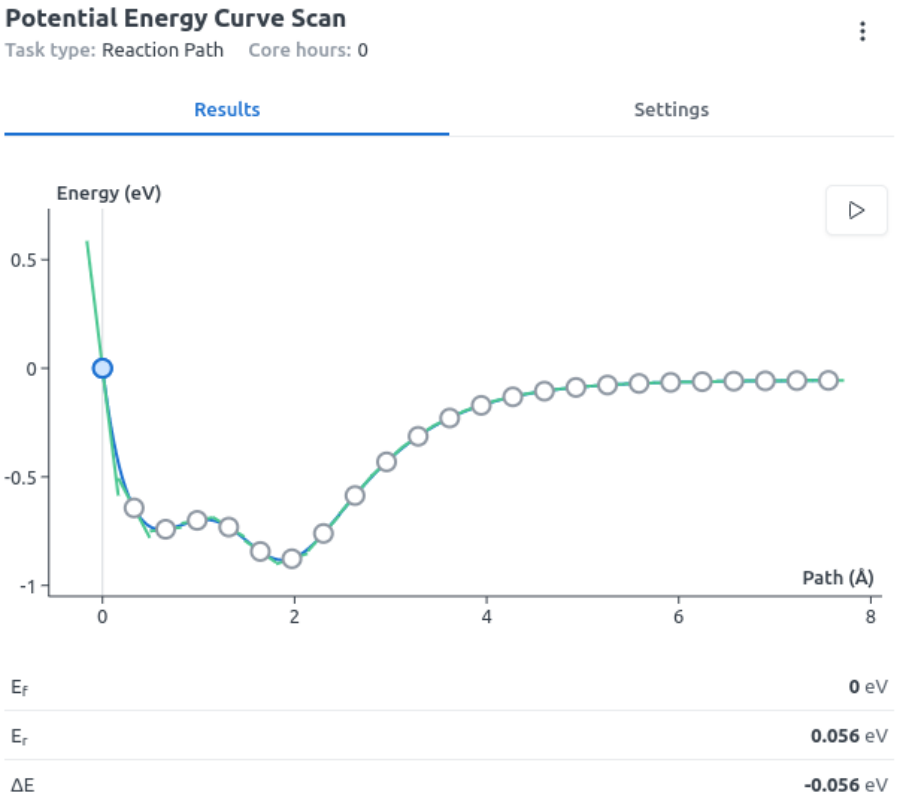
Potential Energy Curve Scan
Task type: Reaction Path
Core hours: 0
Results
Settings
Energy (eV)
0.5
0
-0.5
-1
0
2
4
6
8
Path (Å)
$E_F$
0 eV
$E_r$
0.056 eV
ΔE
-0.056 eV

Figure 2:

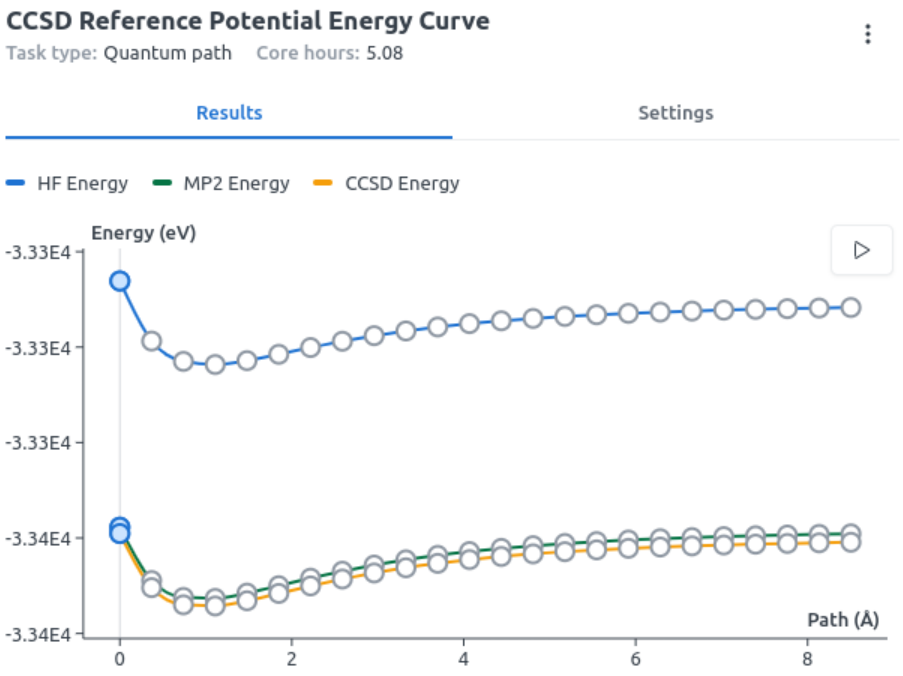
CCSD Reference Potential Energy Curve
Task type: Quantum path
Core hours: 5.08
Results
Settings
HF Energy
MP2 Energy
CCSD Energy
Energy (eV)
-3.33E4
-3.33E4
-3.33E4
-3.34E4
-3.34E4
Path (Å)
0
2
4
6
8

Figure 3:

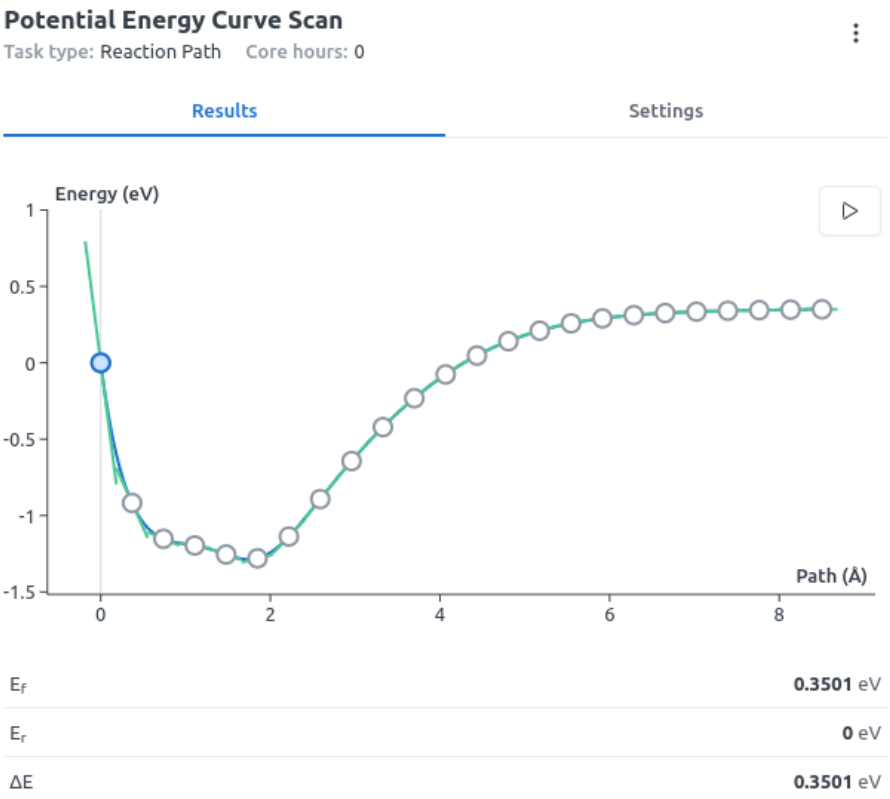
Potential Energy Curve Scan
Task type: Reaction Path
Core hours: 0
Results
Settings
Energy (eV)
1
0.5
0
-0.5
-1
-1.5
0
2
4
6
8
Path (Å)
$E_f$
0.3501 eV
$E_r$
0 eV
ΔE
0.3501 eV

Figure 4:

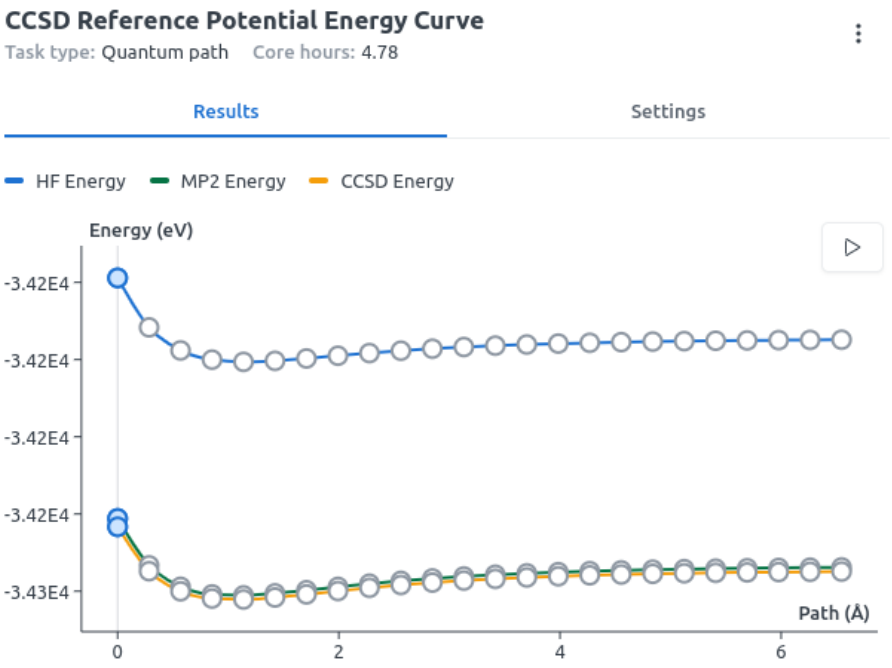
CCSD Reference Potential Energy Curve
Task type: Quantum path
Core hours: 4.78
Results
Settings
HF Energy
MP2 Energy
CCSD Energy
Energy (eV)
-3.42E4
-3.42E4
-3.42E4
-3.42E4
-3.43E4
Path (Å)
0
2
4
6

Figure 5:

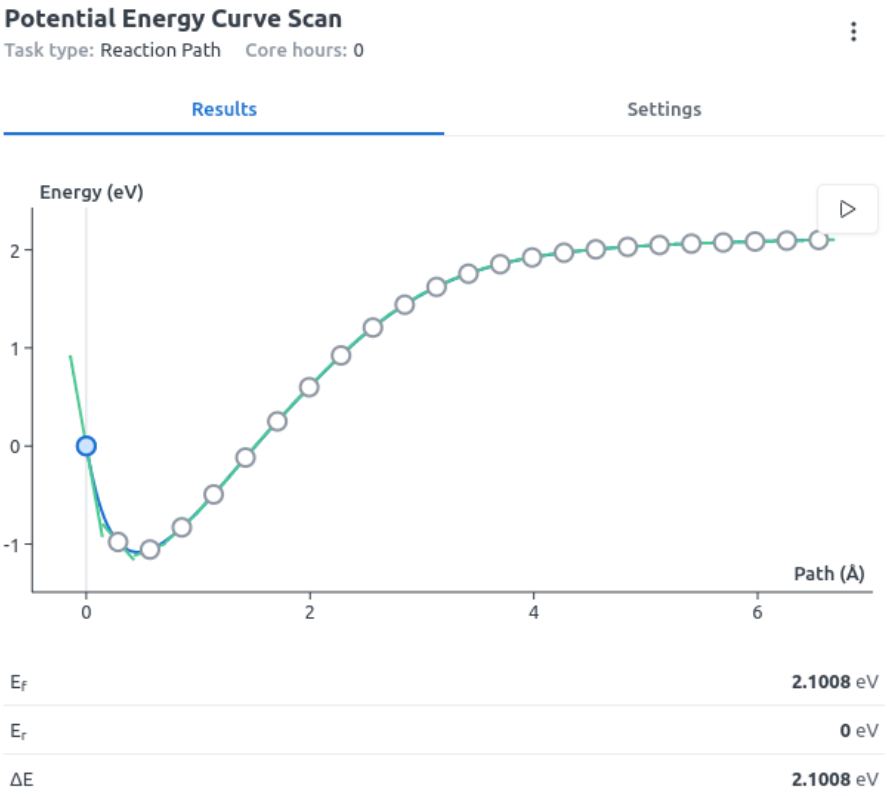
Potential Energy Curve Scan
Task type: Reaction Path
Core hours: 0
Results
Settings
Energy (eV)
2
1
0
-1
Path (Å)
0
2
4
6
$E_f$
2.1008 eV
$E_r$
0 eV
ΔE
2.1008 eV

Figure 6: