

Big Data & Quantum Mechanics: DFT Training

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1 Overview

The introductory project involves calculating the adsorption energy of a carbon monoxide (CO) molecule on a platinum (Pt) surface defined by the (111) Miller index. This system is commonly referred to as CO* on Pt(111), or CO*-Pt(111). The adsorption energy will be computed using the quantum-mechanical method of density functional theory (DFT), which will require utilization of the PACE supercomputing cluster. The adsorption energy will be “converged” with respect to two numerical simulation parameters: k -point sampling and plane-wave cutoff. This will require a total of more than 100 DFT calculations, so students will be introduced to challenges that arise even in organizing “small” data. The exercise will follow a group-maintained tutorial: <https://app.tetra.co/teams/medfordgroup/pages/calculating-adsorption-energies-a-crash-course>, and improvement of this documentation is a key part of the exercise.

2 Goals

2.1 Midterm

2.1.1 Ideal Goal (A+)

DFT calculations of a single adsorption energy with Quantum Espresso along with associated Pt+CO, Pt(111), and CO structures.

Deliverable: Adsorption energy with (4,4,1) k -points and 400 eV planewave cutoff, plus associated ‘.traj’ files. Comparison of adsorption energy to independent calculations from other teammates or prior years.

2.1.2 Expected Goal (A)

Calculations of adsorption energy with EMT along with associated Pt+CO, Pt(111), and CO structures.

Deliverable: Adsorption energy with plus associated ‘.traj’ files.

2.2 Final

2.2.1 Ideal Goal (A)

DFT calculations of adsorption energy for CO* at Pt(111) at all k -point and plane-wave values compared against prior calculations.

Deliverable: Plots of adsorption energy convergence vs. plane-wave cutoff at all k -points.

2.2.2 Expected Goal (B)

DFT calculation of adsorption energy for CO* at Pt(111) for a single k -point sampling and plane-wave cutoff.

Deliverable: Adsorption energy and percent error compared against at least 2 independent calculations, along with associated ‘.traj’ files.

Approved: _____

A.J. Medford
Sub-team Advisor

Approved: _____

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Sub-team Leader