Zacros Tutorial 3: Energetics Input for CO Oxidation on Pt(100)

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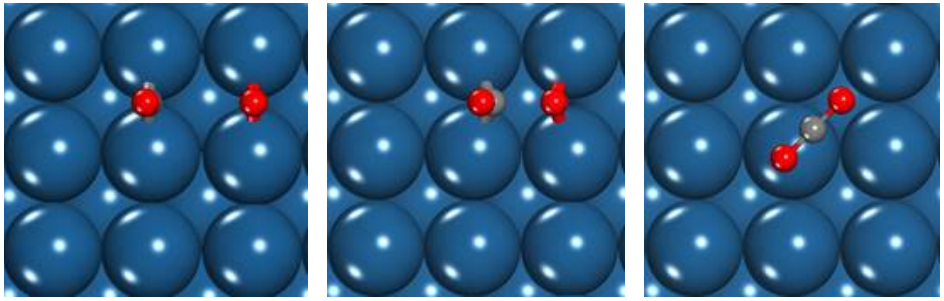
Raw Data from CO Oxidation Calculations

Gas Phase Species	DFT Energy (eV)
O_2 (g)	-7.88
CO (g)	-13.60
CO_2 (g)	-20.76

Clean Slab	DFT Energy (eV)
Pt(100) Clean Surface	-187.15

Adsorbed Species	DFT Energy (eV)
CO Adsorbed on Bridge	-203.11
CO Adsorbed on 4fold	-202.60
O Adsorbed on Bridge	-192.60
O Adsorbed on 4fold	-192.15

"Reactive" states	DFT Energy (eV)
CO+O co-adsorbed (both on Bridge) – (Initial State)	-208.51
Transition State	-207.97
CO_2 loosely adsorbed (vdW) on Pt(100) – (Final State)	-208.11



Initial state Transition state Final state

- We need to convert the energies of this dataset to formation energies before putting them to *Zacros* input files

Calculation of Formation Energies

- First, we need to choose reference states: CO, O_2, Pt(100)
- Then we can calculate formation energies e.g.:

For gas species:

$FE_{CO} = DFTE_{CO} - DFTE_{CO} =$ **0.00 eV**

$FE_{CO_2} = DFTE_{CO_2} - DFTE_{CO} - ½DFTE_{O_2} =$
$-20.76 - (-13.60) - ½(-7.88) =$ **–3.22 eV**

For adsorbed states:

$FE_{CObrg} = DFTE_{CObrg} - DFTE_{Pt(100)} - DFTE_{CO} =$ **–2.36 eV**

$FE_{CO_2vdW} = DFTE_{CO_2vdW} - DFTE_{Pt(100)} - DFTE_{CO} - ½DFTE_{O_2}$
$=$ **–3.42 eV**

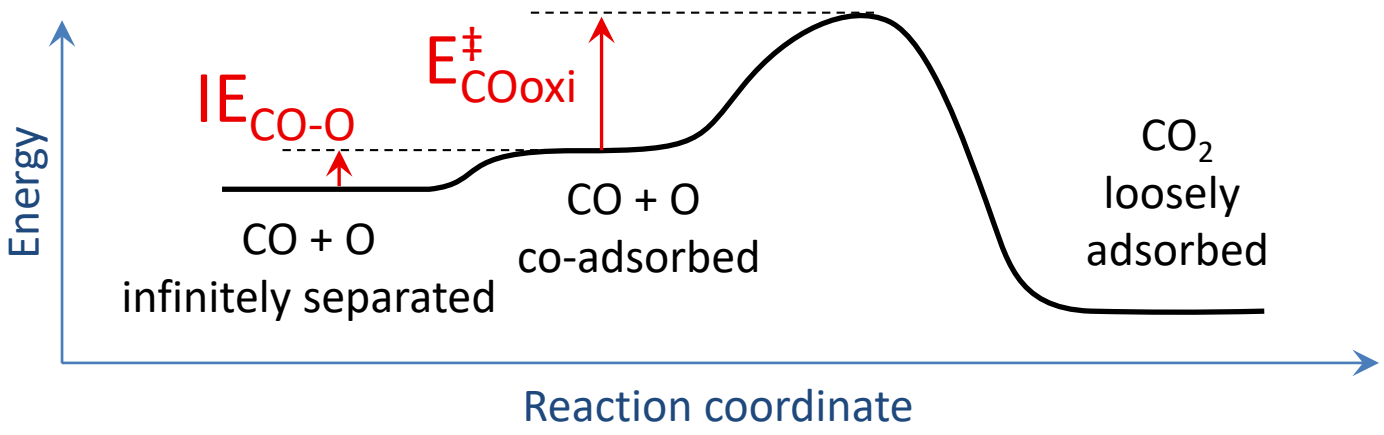
Calculation of Interaction & Activation Energies

- Next we will calculate the interaction energy between CO and O in the co-adsorbed state:

$$IE_{CO\text{-}O} = FE_{CO+O\text{-}coads} - FE_{CO} - FE_{O} = 0.05 \text{ eV}$$

- Finally, the activation energy of the CO oxidation event:

$$E^{\ddagger}_{COoxi} = FE_{COO\text{-}TS} - FE_{CO+O\text{-}coads} = 0.54 \text{ eV}$$



Activity

- Calculate the formation energies of all other species.
- Using the information calculated, create the input files **`simulation_input.dat`** and **`energetics_input.dat`**. For guidance, you can use: the slides of the first tutorial of this workshop, the manual, and the online tutorial: http://zacros.org/tutorials/4-tutorial-1-ziff-gulari-barshad-model-in-zacros
- Use the **`lattice_input.dat`** file created in tutorial 2 and check that *Zacros* parses these files (you should get no errors for these files, but you are expected get an error that the mechanism input file is missing).