CO2/Bi(111)

Theodoros E. Panagiotakopoulos

UCF | Department of Physics

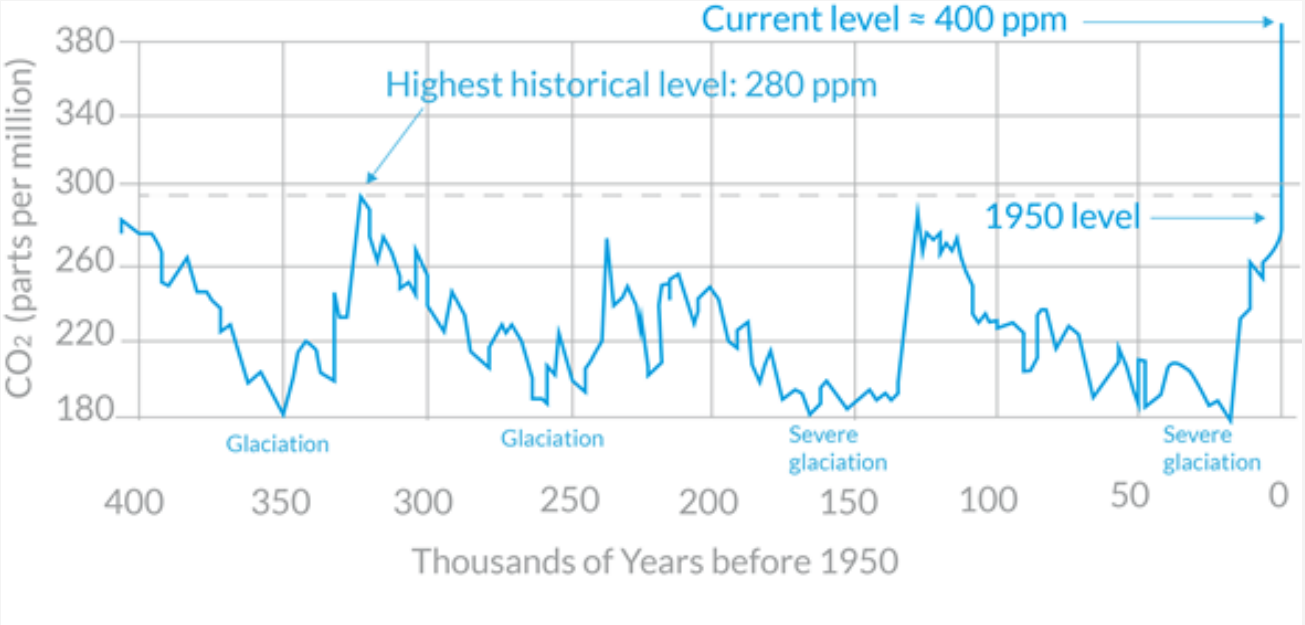
UNIVERSITY OF CENTRAL FLORIDA

Overview

Motivation

(CO2) emissions

- The world watches out for carbon dioxide (CO2) emissions. The excess gas is the main cause of global warming due to the greenhouse effect.



[1]

[1] U.S. NOAA (National Oceanic and Atmospheric Administration)

Computational Details

Input paremeters

- DFT, employing the projector-augmented wave (PAW) and the plane-wave basis set
- PBE exchange correlation function
- Kinetic energy cut-off: 500 eV
- Electronic convergence threshold: 10^{-6} eV
- Supercell: 6x6x6 Bi(111) slab,
  1. CO2 atoms on both sides
  2. Vacuum of 15 (For 1 ML Pb coverage: 216 Bi, 2 C, 4 O)
- Kpoint mesh: (1x1x1) for relaxation

CO2 configurations

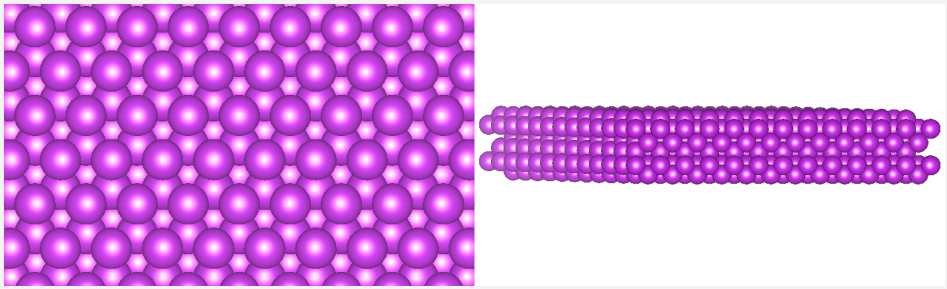
CO2

- There are two configurations for CO2:
  1. Two oxygen atoms up
  2. Two oxygen atoms down

Figure 1: First configuration

Figure 2: Second configuration

Absorb the two configurations of CO2 on Bi(111)



CO2/Bi(111) configurations

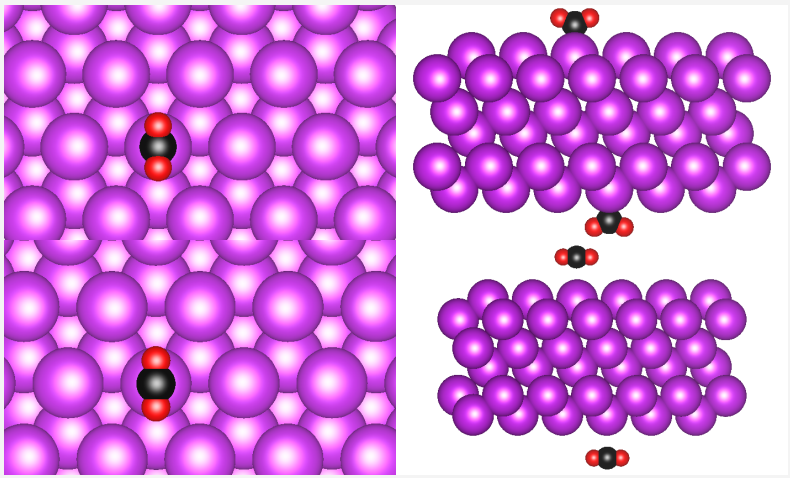


Figure 3: First configuration

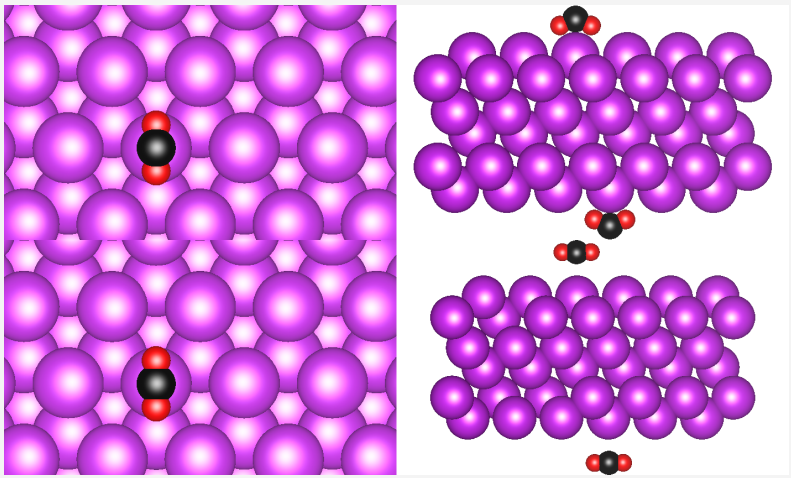


Figure 4: Second configuration

CO2/Bi(111) absorbtion

- Calculations were pefromed for 0, 2 and 4 electrons
- It seems that CO2 is not being on Bi(111)

CO2/Bi(111) configurations

Why charge?

- CO2 is stable molecule and hard to adsorb on anything
- Adsorption happens only if it forms a v shape configuration
- This can happen only if CO2 receive electron to its π antibonding orbital
- So charging the surface increase the amount of electron transferring to pi* orbital

CO2/Bi(111) configurations

CO2

- CO2 could not be absorbed on the surface
- two configurations of COOH used
- COOH may be absorbed on Bi(111)[1] so H will then be removed

Figure 5: First configuration

Figure 6: Second configuration

COOH/Bi(111) configurations

COOH

- Calculations were pefromed for 0, 2 and 4 electrons
- We were able to absorb COOH on Bi(111)

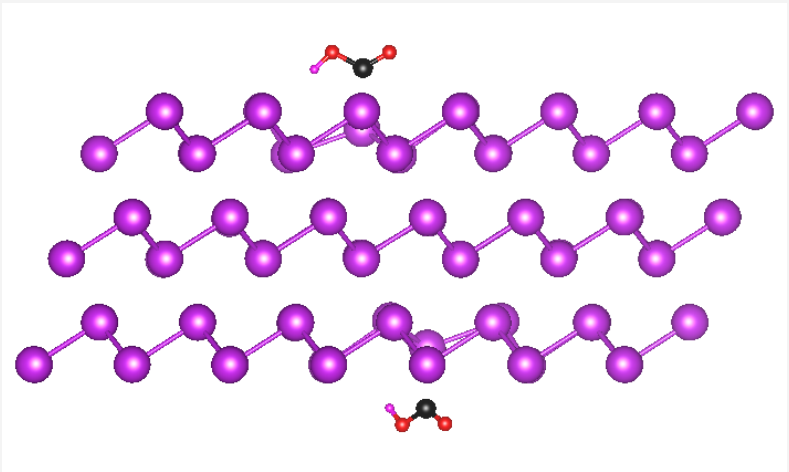


Figure 7: COOH absorbed on Bi(111)

- Next we remove H and we add cat-ion $NH4^{+}$

$CO_2 + NH_4^+/Bi(111)$

$CO_2 + NH_4^+/Bi(111)$

- After trying many configurations finally we get the one where CO_2 stays bended on Bi(111)
- Calculations were performed 1, 3 and -1 electrons
- C was initially constrined
- after relaxation, constraints were removed and new relaxation calculations performed

CO2 + $NH4^+$/Bi(111)

CO2 + $NH4^+$/Bi(111)

- CO2 is bended for calculations with 1 e^- added since this number gives aproximately the potential of -1 eV used in experiments

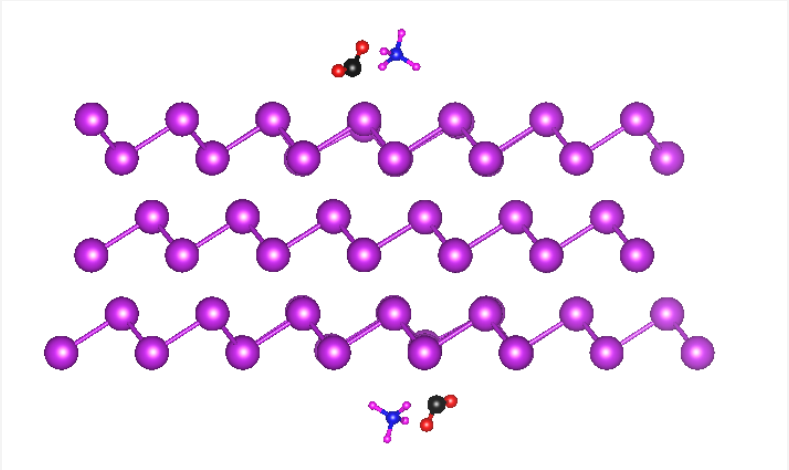


Figure 8: CO2 & $NH4^+$/Bi(111) after relaxation

Next Steps

Next Steps

- Target potential calculations are running for $NH4^+$ directly above C atoms
- $NH4^+$ will be removed and see if CO2 stays bended by setting the target potential equal to -1 eV
- Use H_2O instead of $NH4^+$ and check if we can use H_2O instead

References

Wooseok Oh, Choong Kyun Rhee, Jeong Woo Han, and Bonggeun Shong.
Atomic and molecular adsorption on the bi (111) surface: insights into catalytic co2 reduction.
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