Multiscale Machine-Learning and DFT Study of CO_2 Hydrogenation on Zn/ZnO–Cu Interfaces for Reducing Greenhouse Gas Emission

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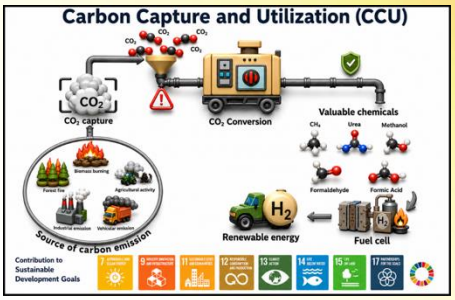
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Abstract

The discrepancy in the catalytic behaviours in ultra-high vacuum vs. realistic gas environments, known as "*pressure gap*", has been a long-standing challenge in the field of surface science. Here, we investigate the morphology of ZnO clusters on Cu surface. We compare the activity of various ZnO morphologies towards CO2 hydrogenation reactions.

Introduction

- Global warming is largely driven by the high levels of CO_2 released into the atmosphere from burning fossil fuels.
- So, how can we reduce these emissions and lessen the greenhouse effect?
- One promising solution is converting CO_2 into valuable compounds through hydrogenation, using affordable copper-based (Cu) catalysts.

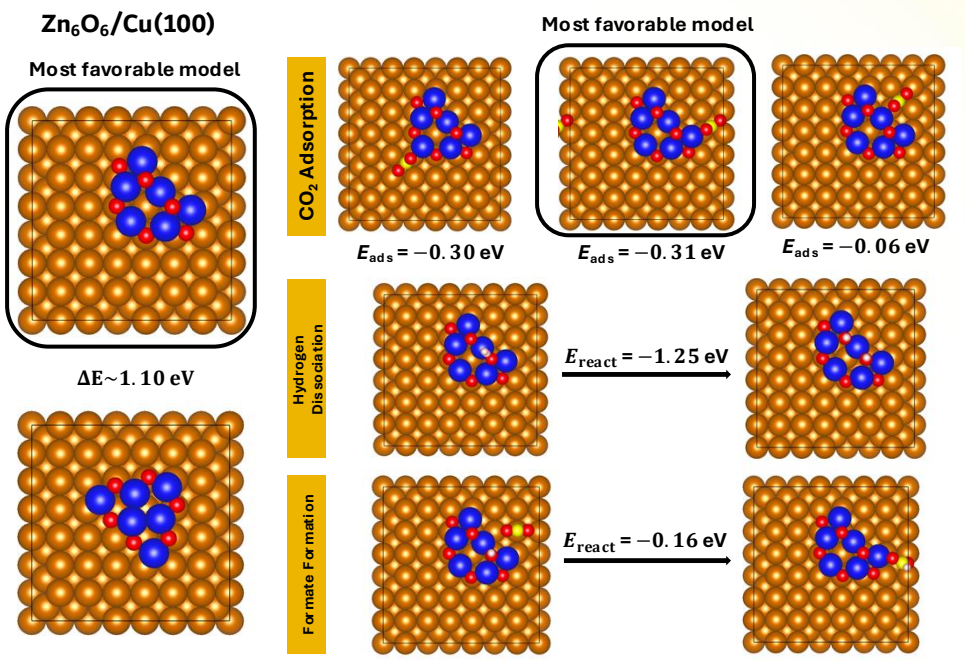


Computational Methods

- 7×7 supercell of slab model
- 2×2×1 of *k*-points
- Energy cutoff for the plane-wave basis set is 450 eV
- PBE-D3 exchange-correlation functional
- Spin-polarized calculations

VASP

Computational Results



Output

- Various ZnO cluster morphology on Cu(100) surface.
- Creating datasets for the CO_2 hydrogenation process on ZnO/Cu(100).

Conclusions

- 3D-like ZnO cluster morphology is more stable.
- CO_2 is activated at the interface between ZnO cluster and Cu surface.
- The ZnO cluster lowers the reaction energy (E_{react}) of the CO_2 hydrogenation step.

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