Theoretical approach for enhancing ZnO-based sensors

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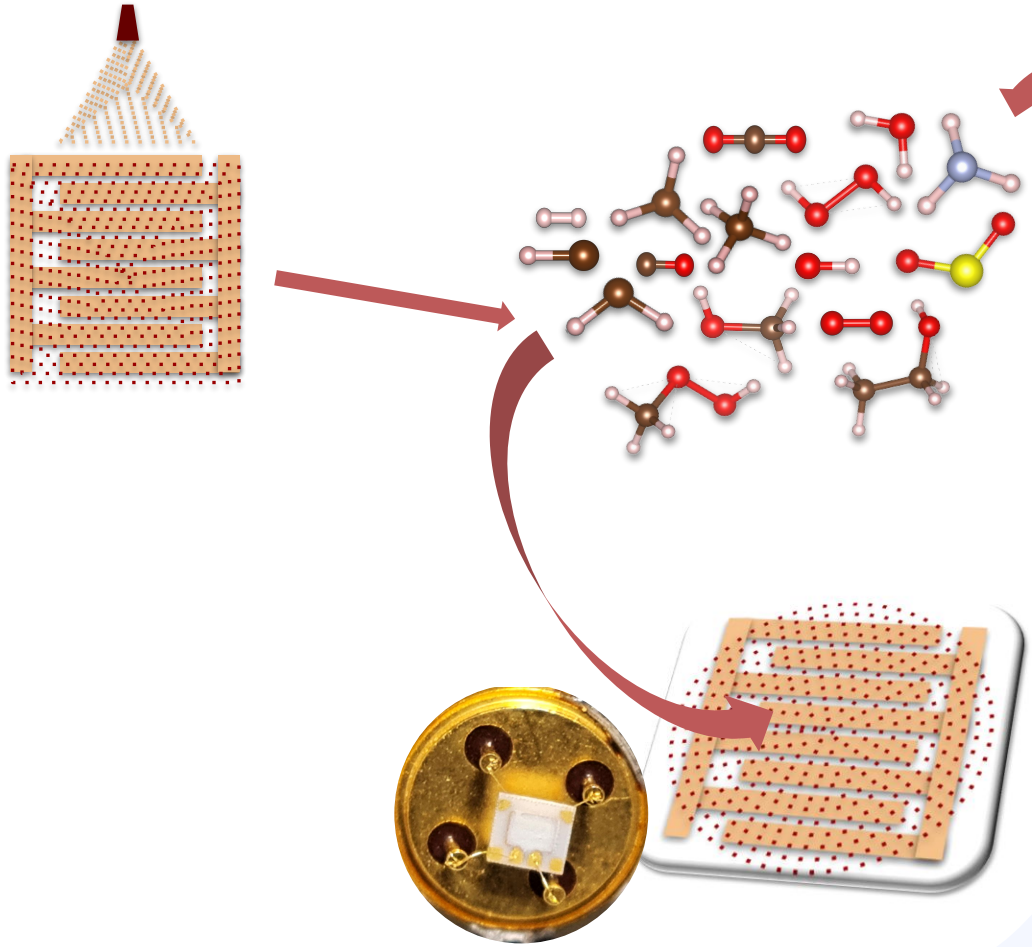
Theoretical Study of Materials

Motivation

Devices that transmit environmental data for real-time monitoring and analysis



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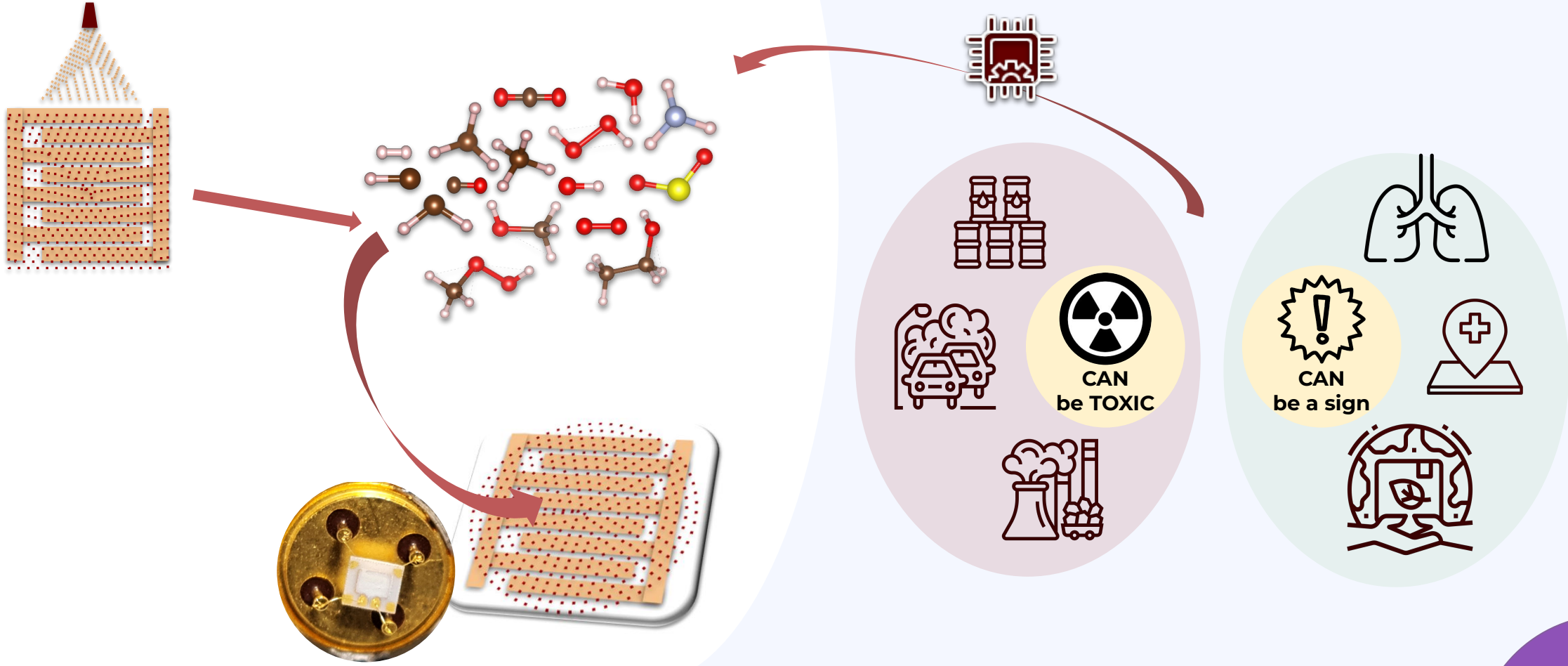


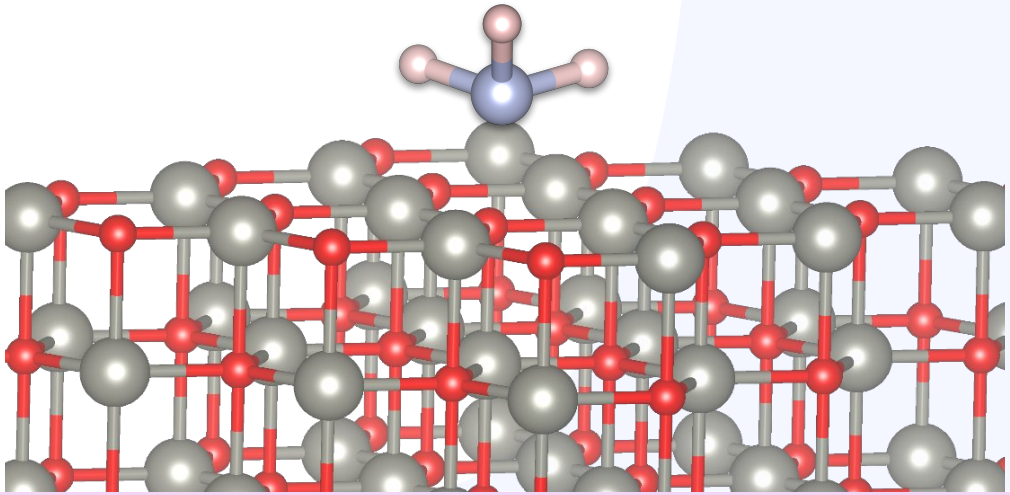
Sensor Activity

Adsorption step: $ZnO + NH_3$

Intermediate state: $H_3N\text{-}ZnO$

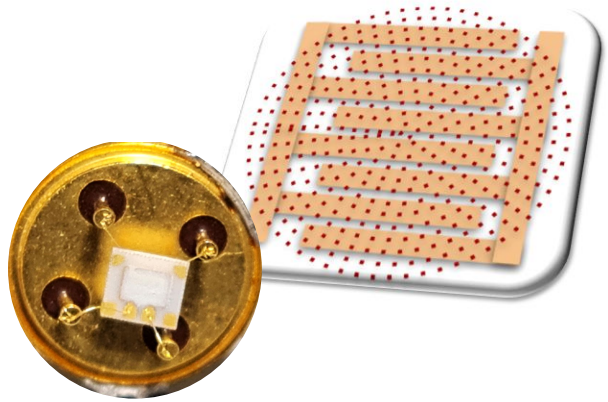
Transition state: $H^+ + H_2N\text{-}ZnO$

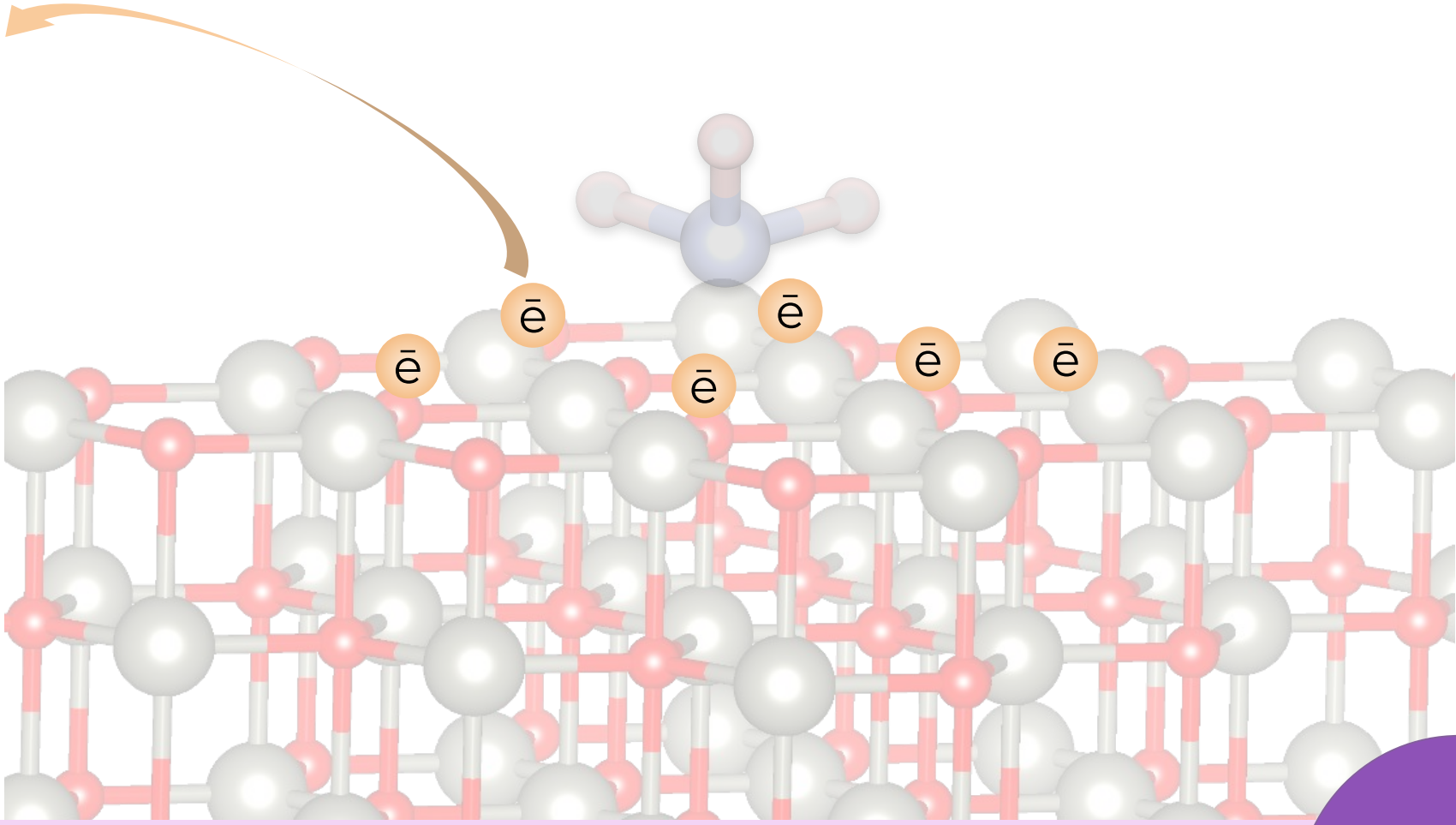
Charge transfer: $H^+ + (H_2N)^{2+}\text{-}ZnO + 6e^-$



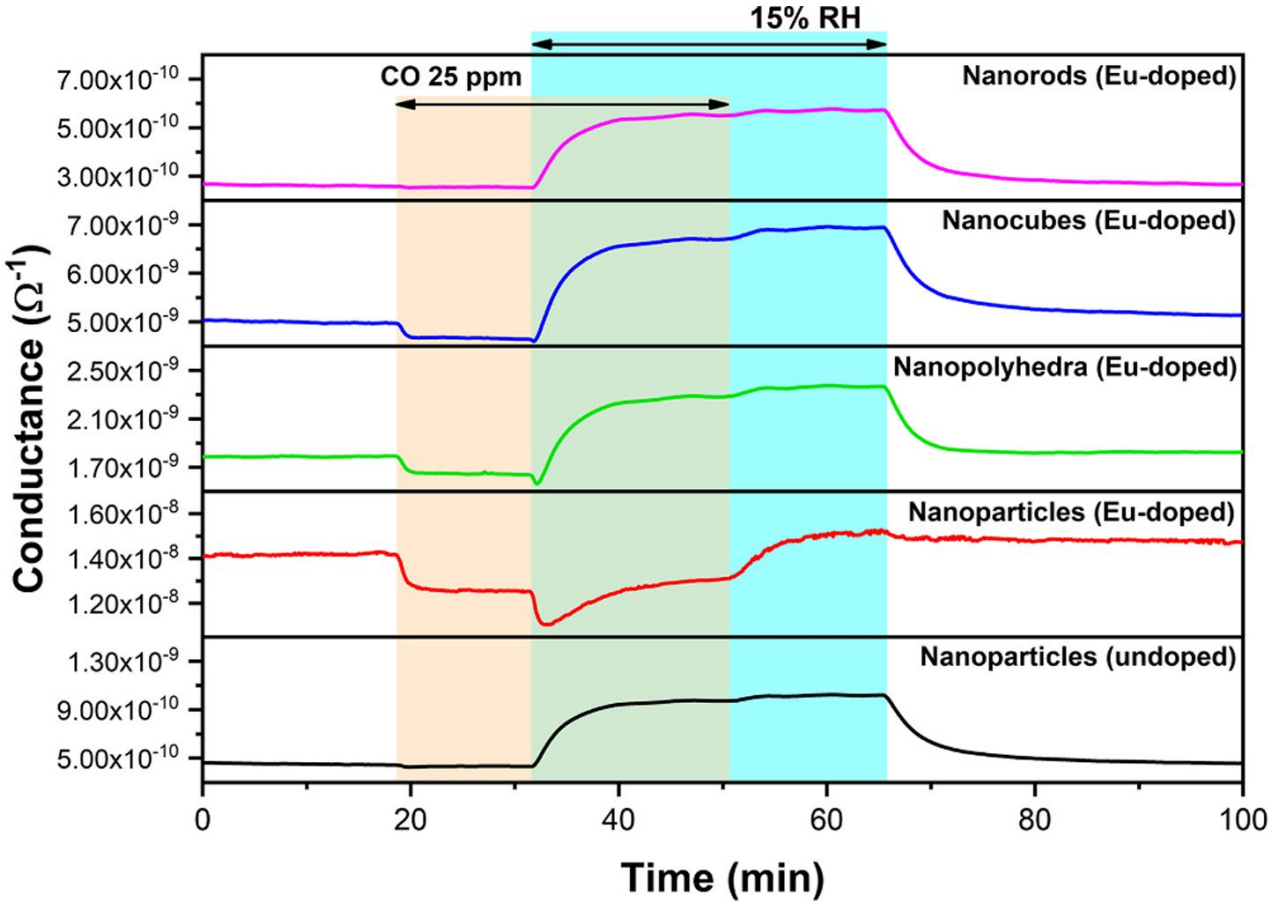
Sensor Activity

- Electrical signal
- Conductance
- Catalyst





Humidity Influence



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- Formation of hydrogen bonds between the gas and water molecules on the surface or between water and the surface
- Humidity becomes an important issue for gas sensors!
- Competition between H_2O and the gas?
- Can we recovery the sensor response?

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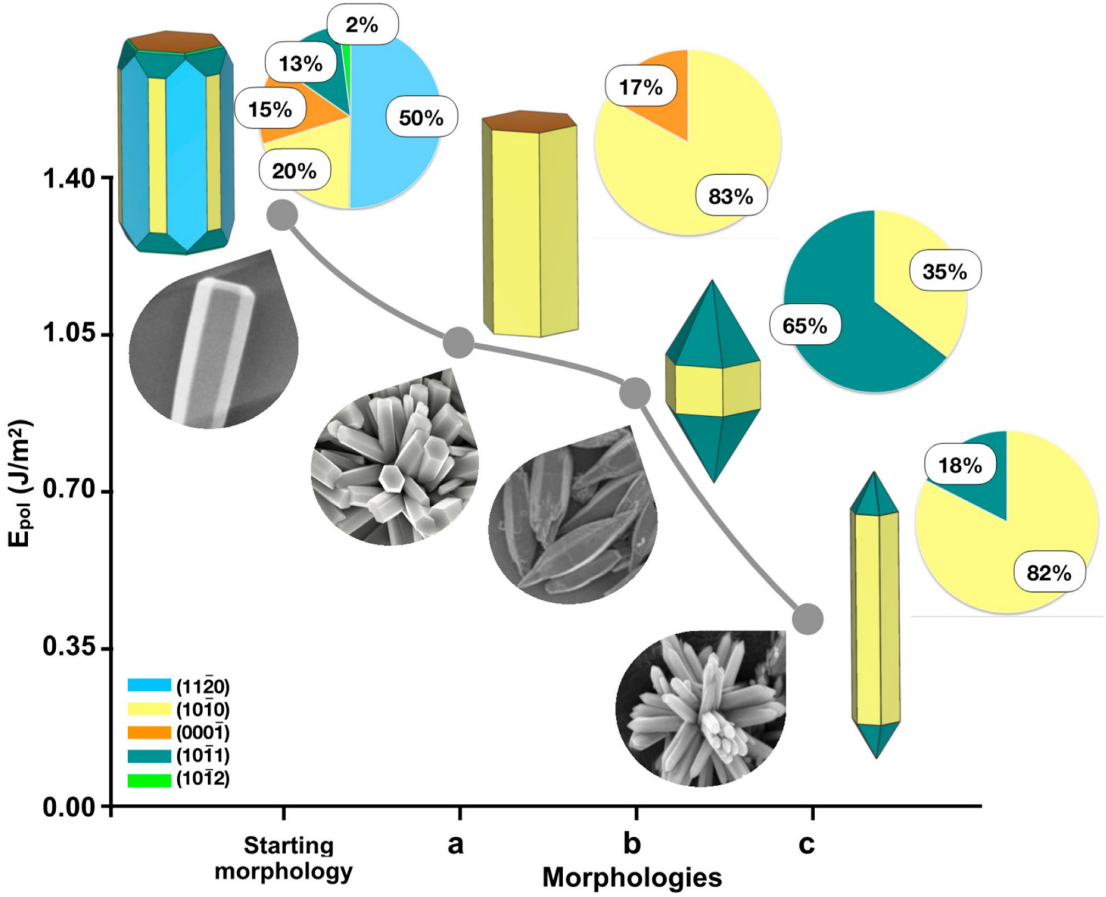
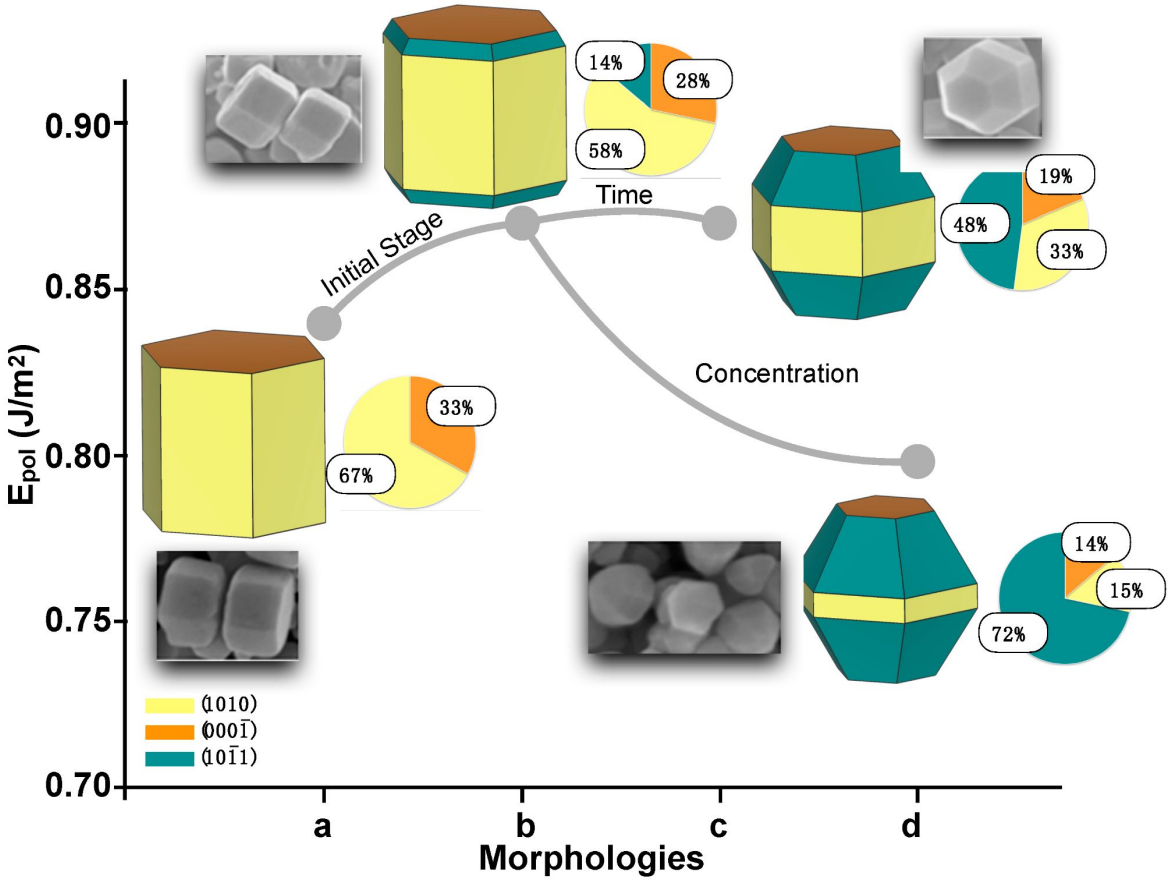
ZnO surfaces (0001) (1010) (1011)





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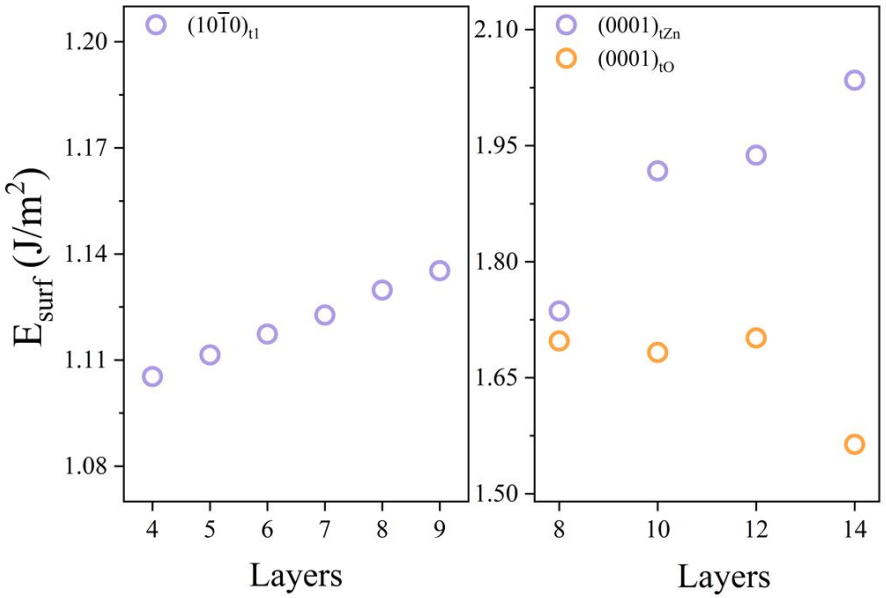
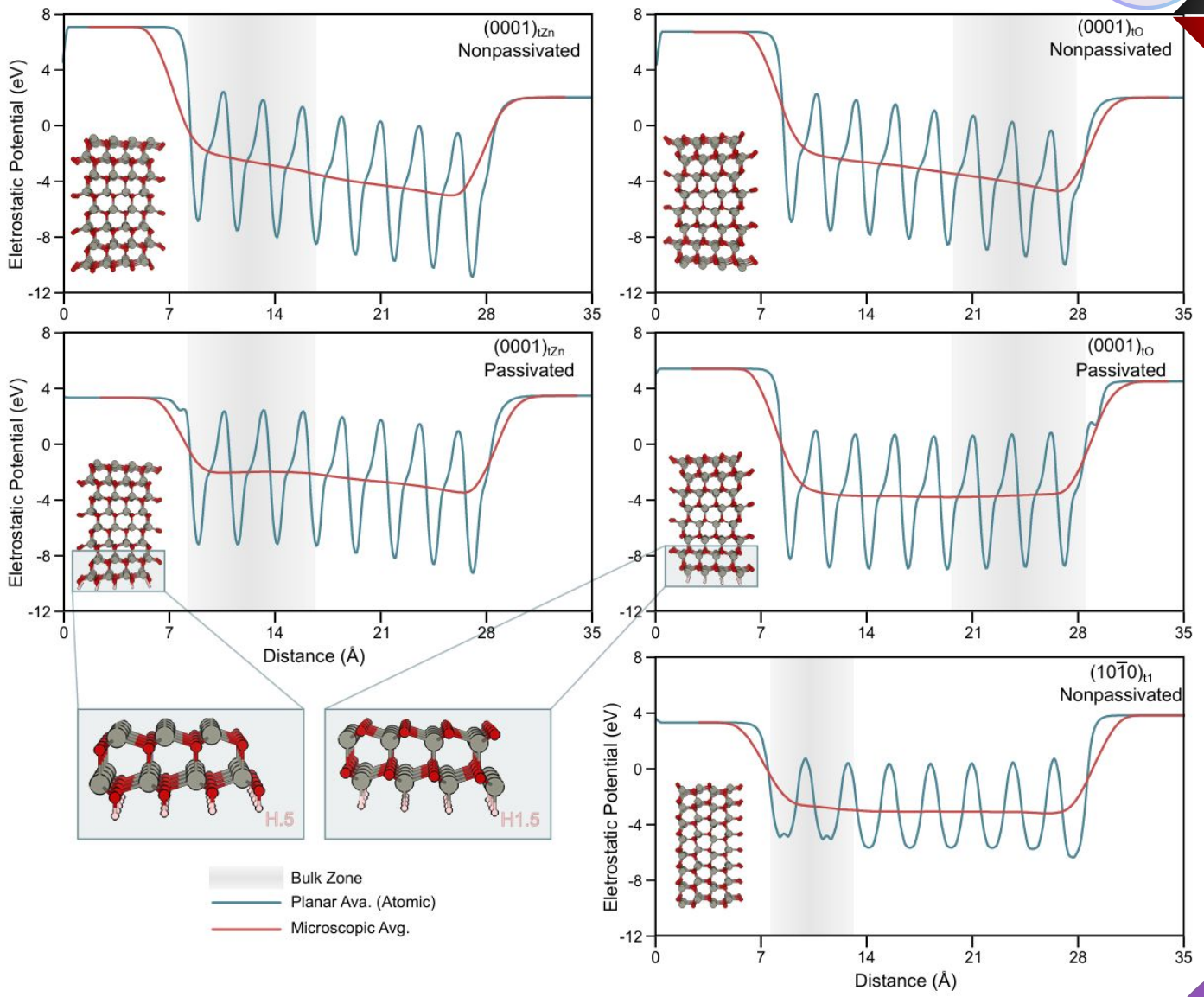
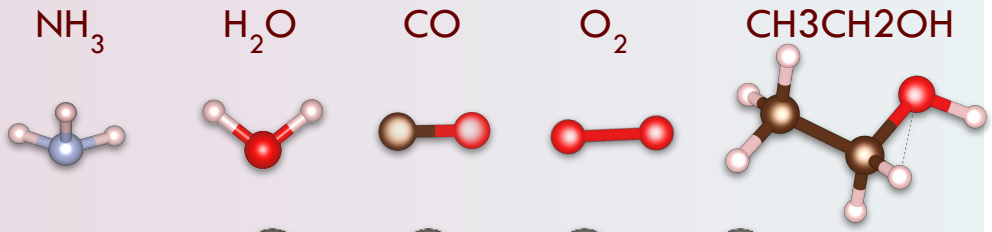
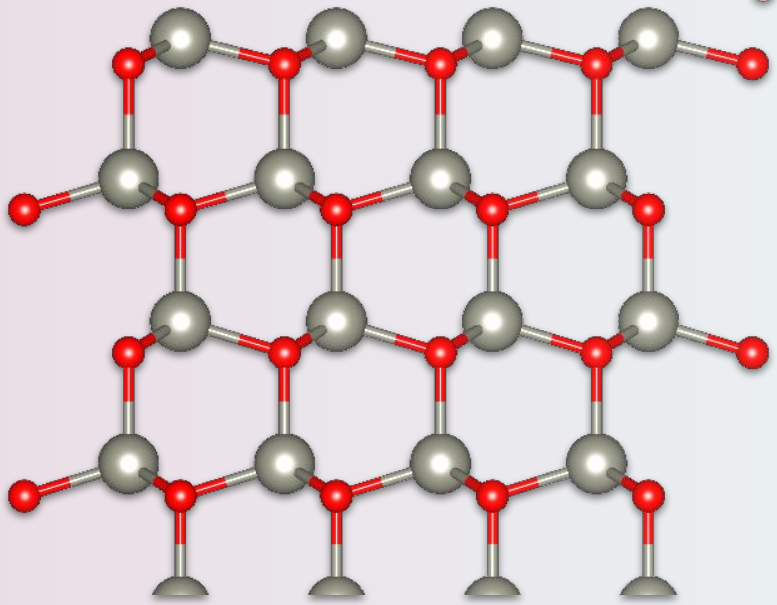
ZnO surfaces





Adsorption





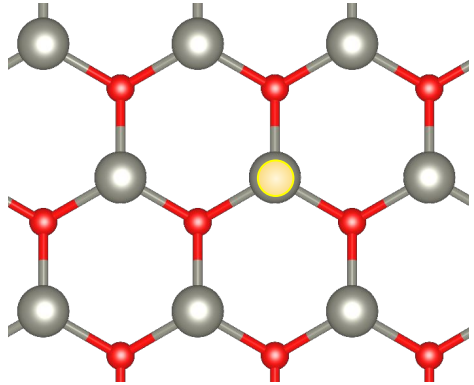
Zn

O

Adsorption Energy

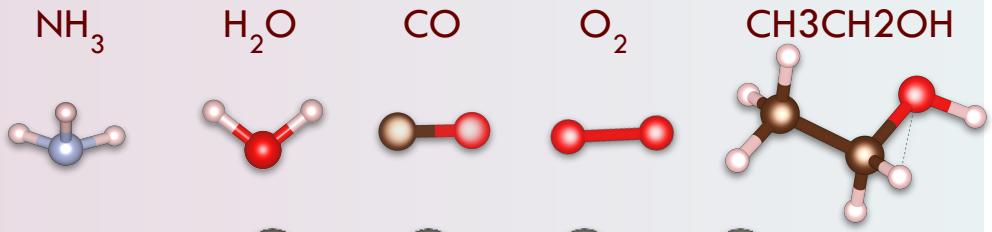
$$E_{ads} = E_{tot}^{mol/sensor\text{-}OPT} - \left(E_{tot}^{mol\text{-}OPT} + E_{tot}^{sensor\text{-}OPT}\right.$$

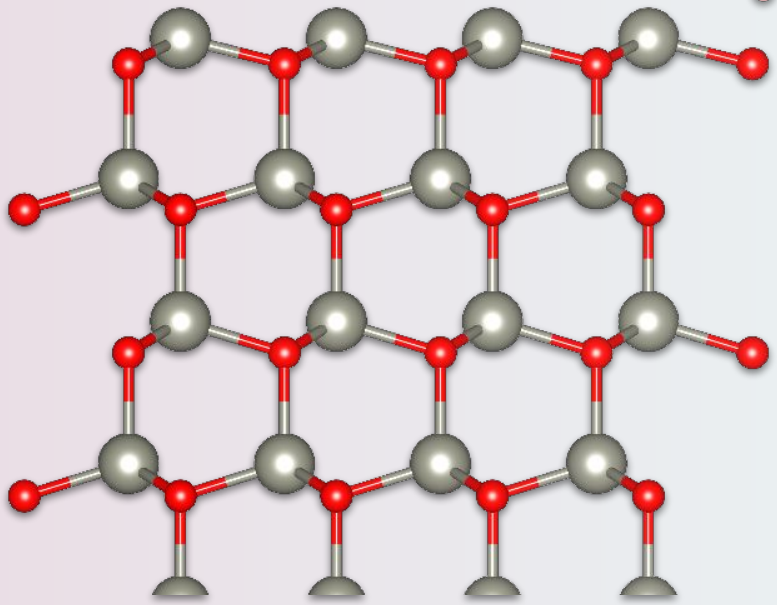
Adsorption Sites



TOP

Adsorption





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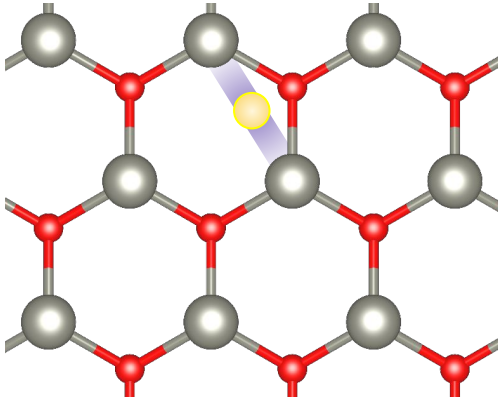
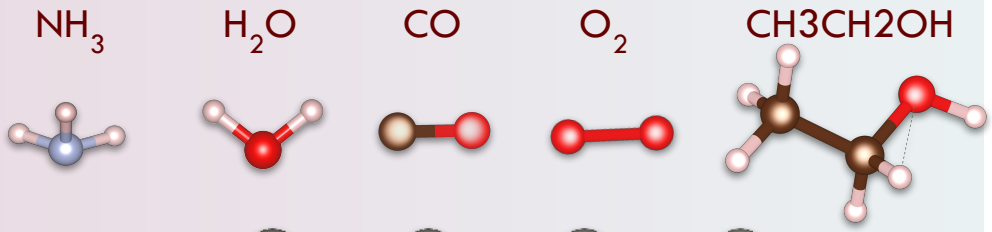
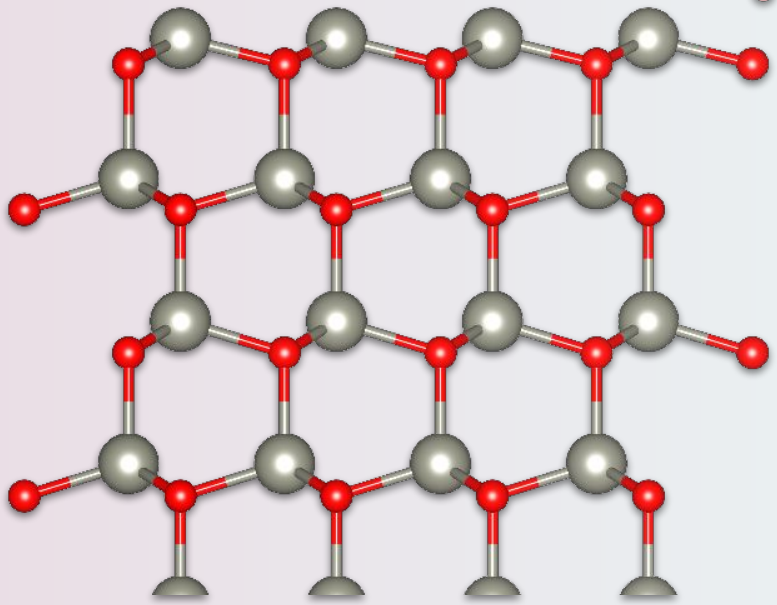
Adsorption Sites



BRIDGE

Adsorption





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Adsorption Energy

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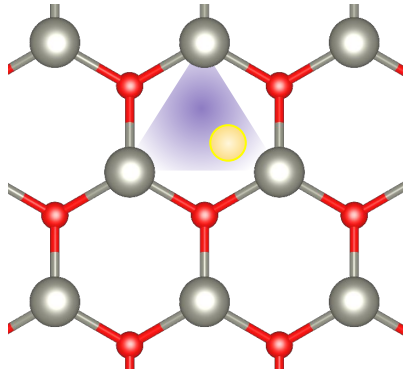
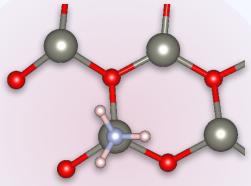
Adsorption Sites



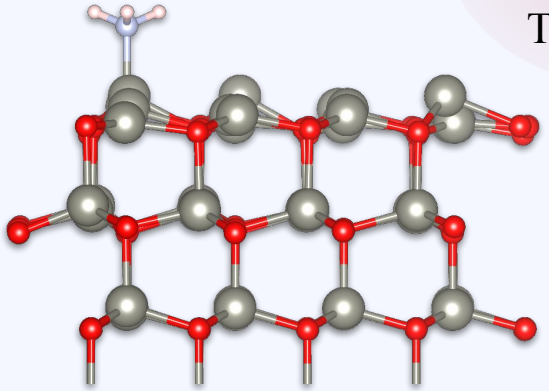
HOLLOW

Adsorptions

NH_3

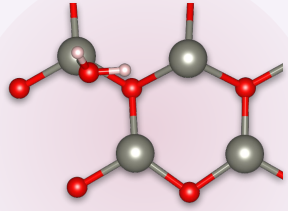


Top View

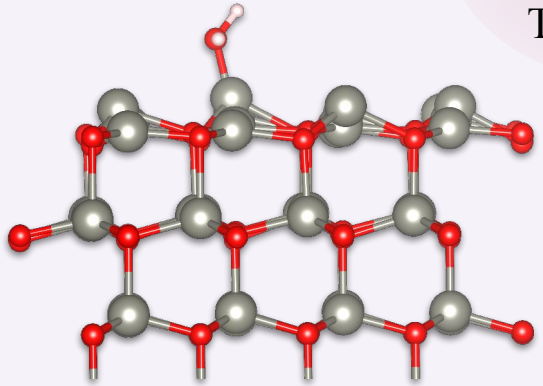


NH_3	TOP
E_{ads} (eV)	-0.87
D_{mol_surf} (Å)	2,09
Atoms	N - Zn

H_2O



Top View

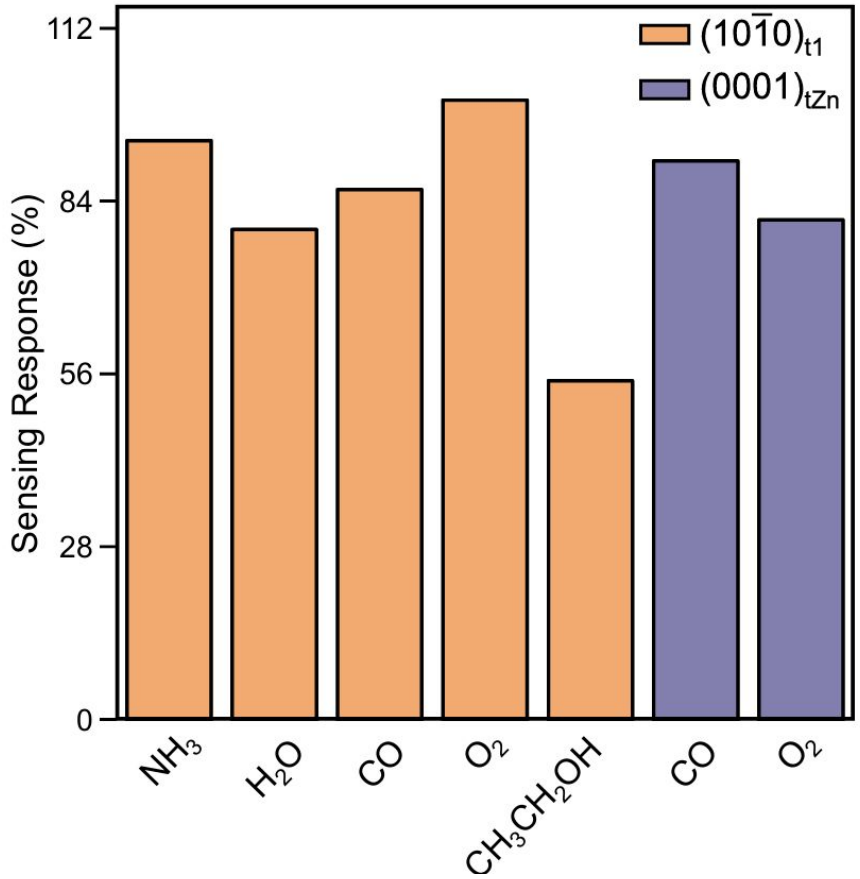


H_2O	TOP
E_{ads} (eV)	-0.64
D_{mol_surf} (Å)	2,10
Atoms	O - Zn

Adsorptions

$$S(\%) = \left(\frac{\sigma_{ads} - \sigma_{surface}}{\sigma_{ads}} \right) 100(\%)$$

$$\sigma \propto exp\left(\frac{-E_{gap}}{2k_B T} \right)$$



Humidity Influence

- Analyse the impact of the morphology on the gas interaction
- Improve the sensor sensitivity accounting for the effect of humidity
- Determine the surface interactions

(0001) (1010) (1011)

- Study other surfaces and co-adsorptions

Acknowledgments

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