

Computational Study on Enhanced CO Sensing Properties of Boron-doped Zn₁₂O₁₂ Nanocluster

Mahnoor Ehsan^a, Fouzia Malik^{a, *}

^aSchool of Interdisciplinary Engineering and Science (SINES), National University of Sciences and Technology (NUST)

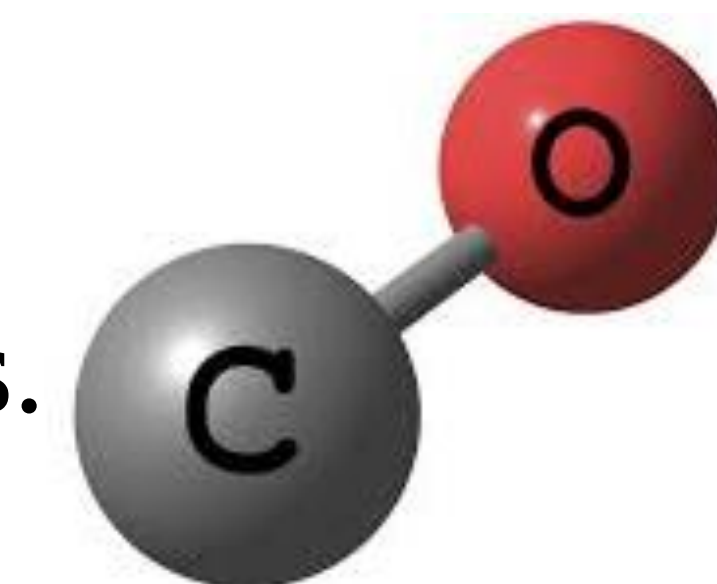
Sector H-12, 44000 Islamabad, Pakistan

*Email: fouzia@sines.nust.edu.pk



1 PROBLEM STATEMENT

The silent Killer



No Taste
No Color
No Smell

CO gas is the product of incomplete combustion of carbon containing materials. CO is a **threat** to human life and environment pollutant.

Nanocluster Zn₁₂O₁₂ is a metal oxide semiconductor based chemical gas sensor. It rationalizes the resistance behavior upon CO adsorption. Doping manipulates the geometry of nanocluster making it highly sensitive to CO gas based on change in conductivity due to presence of CO molecules.

Significance:

- Micro/nano forms
- Stable cluster
- Easily prepared
- Non-toxic

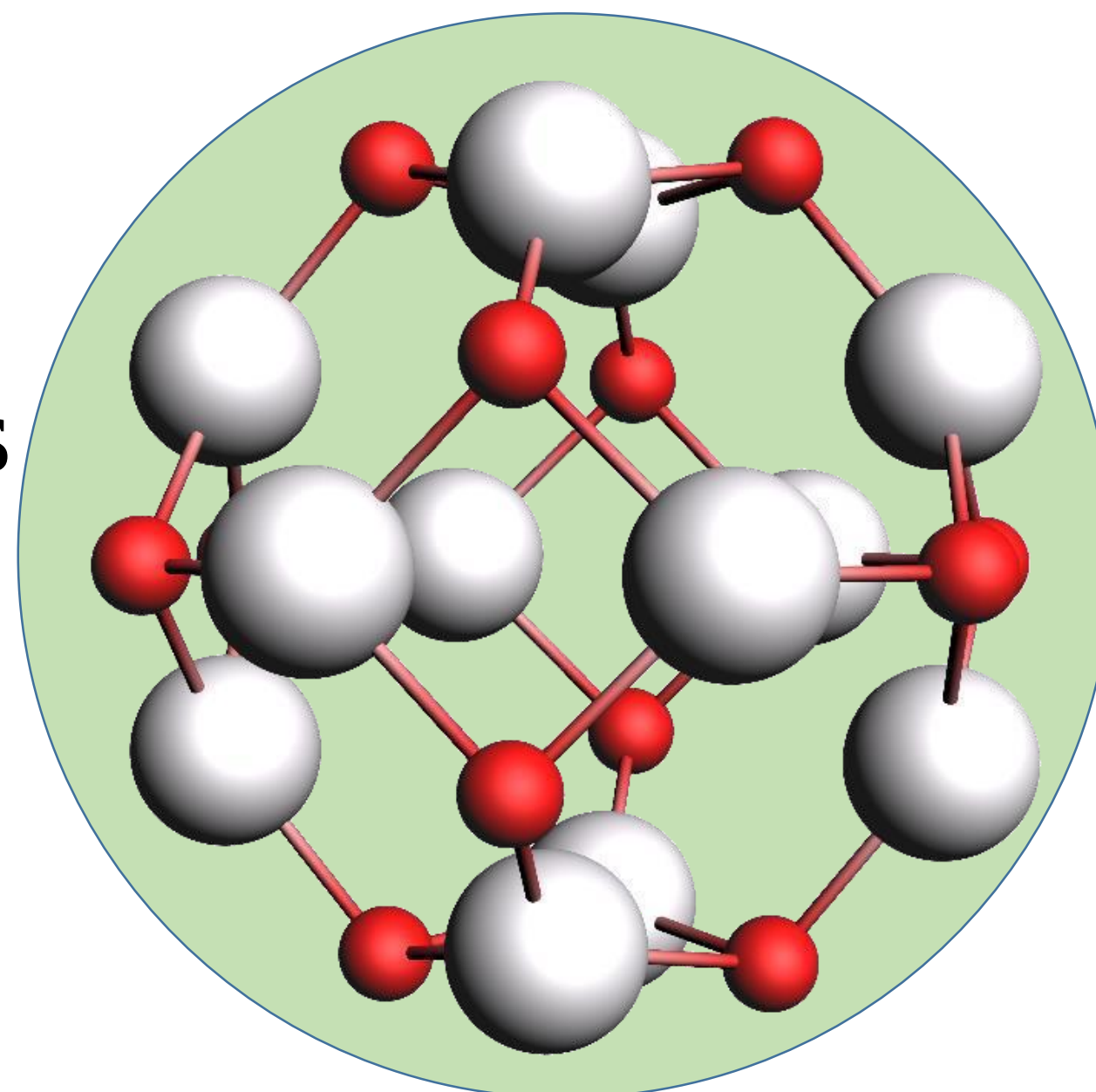
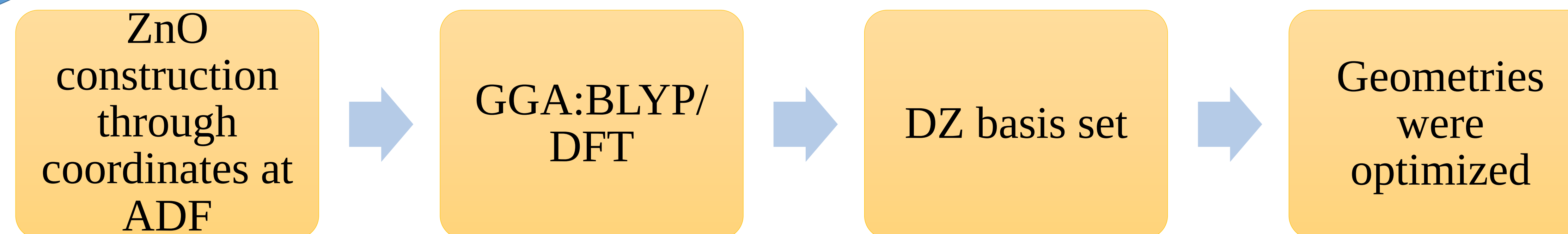


Fig 1: Optimized geometry of Zn₁₂O₁₂ nanocluster

- Favorable morphology
- Wide direct band gap (3.4-3.7 eV)
- Good selectivity
- Impurity incorporation improves sensitivity

3 METHODOLOGY

Quantum Chemical Calculation $H\psi=E\psi$



4 RESULTS

S.NO	SYSTEMS	E _{HOMO} (eV)	E _{LUMO} (eV)	E _g =E _{LUMO} -E _{HOMO}	Charge Transfer Q _r (e)	Optimized Energies (eV)	Adsorption Energy E _{ad} (eV)
1	(SPE) Zn ₁₂ O ₁₂	-6.40	-2.79	3.61	-	-81.31	-
2	Zn ₁₂ O ₁₂	-6.27	-4.26	2.01	-	-82.84	-
3	CO@Zn ₁₂ O ₁₂	-6.12	-4.19	1.93	-0.50	-93.78	1.8
4	B-Zn ₁₁ O ₁₂	-4.39	-3.34	1.05	-	-89.77	-
5	CO@B-Zn ₁₁ O ₁₂	-4.37	-3.52	0.85	-0.53	-100.47	2.0

Table 1: Electronic properties

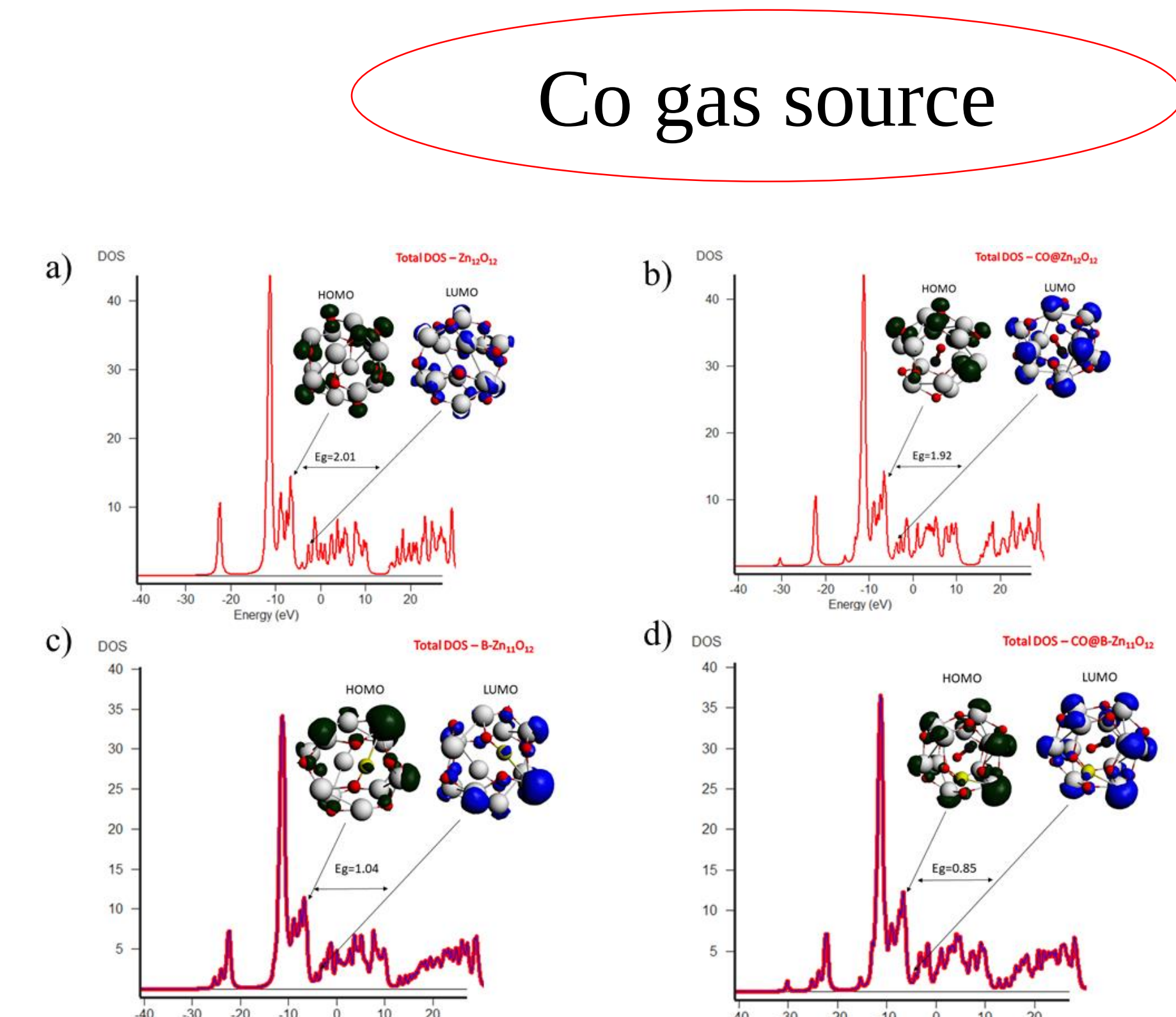


Fig 3: Density of States (DOS)

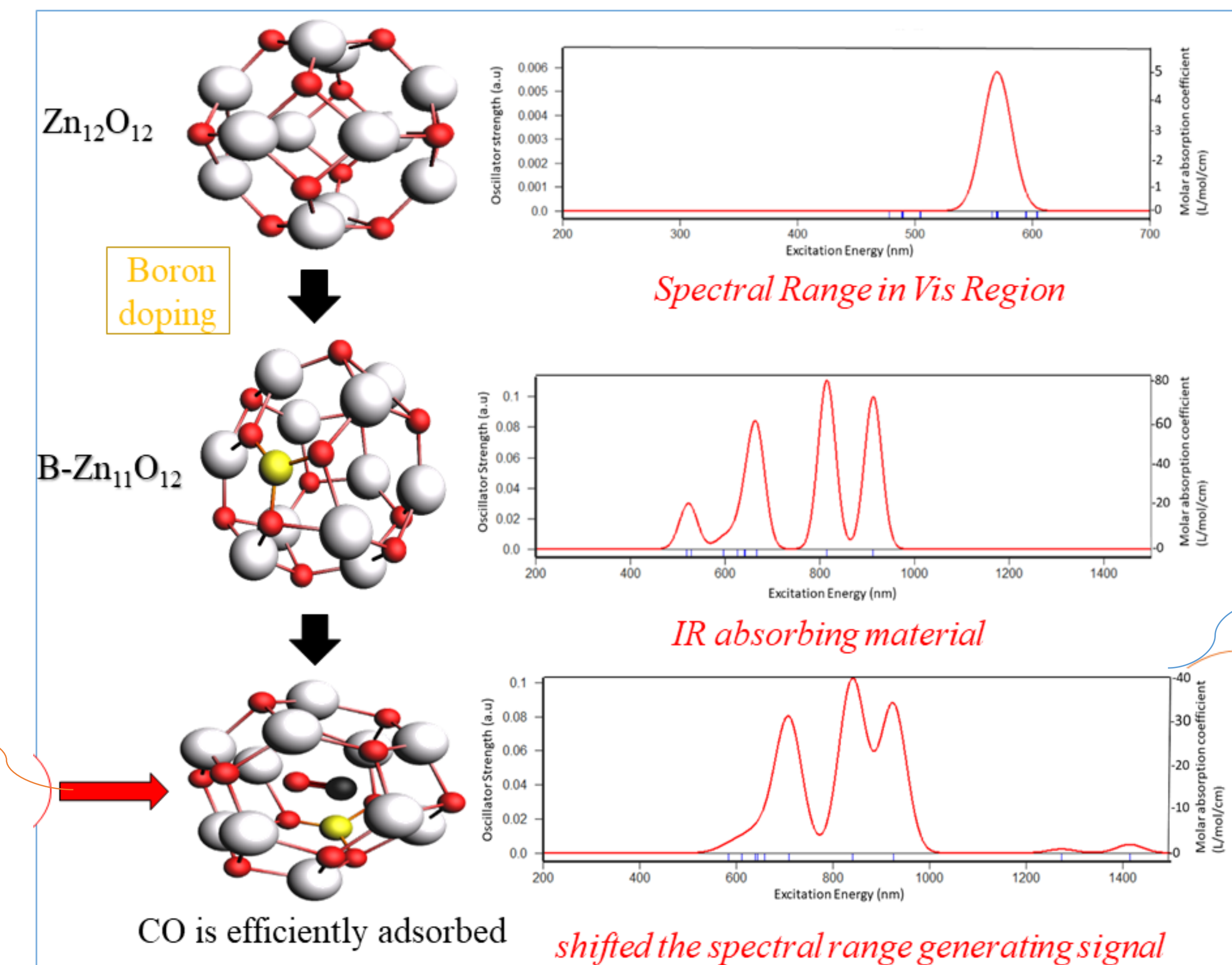


Fig 2: Mechanism based on Spectroscopic property

S.NO	SYSTEMS	ΔS (cal/mole-K)	Cv (J/K)	ΔH (J/mol)	ΔG (J/mol)
1	Zn ₁₂ O ₁₂	205.514	109.844	-7.74096	-8.0034
2	CO@Zn ₁₂ O ₁₂	216.039	122.885	-8.81703	-9.0901
3	B-Zn ₁₁ O ₁₂	210.411	109.828	-8.4412	-8.7004
4	CO@B-Zn ₁₁ O ₁₂	218.946	120.086	-9.45126	-9.7207

Table 2: Thermodynamic properties

5 CONCLUSION

Boron-doped Zn₁₂O₁₂ can be used to develop the new generation of sensitive, accurate and portable gas sensor devices. This research is a computational prototype that may open new doors to expanding nano applications in industry and technology, and more importantly, a potential benefit to human quality of life.

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