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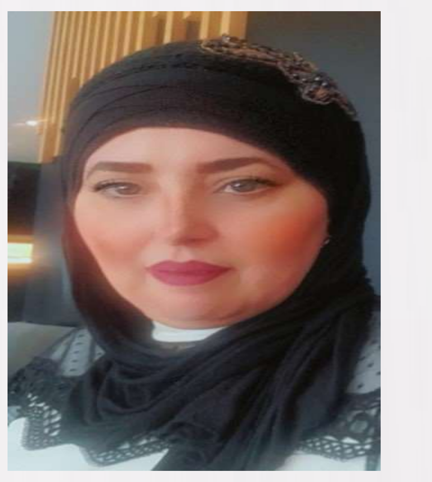

# Study of Chemisorption and Sensing Performance of the Phenytoin Molecule on $Be_{12}O_{12}$ and $GaBe_{11}O_{12}$ Nanocages


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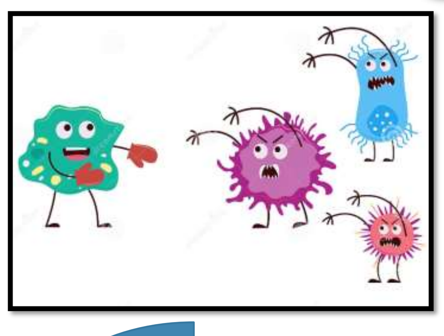
## Introduction



How does the size of the Gan cluster influence the stability, the strength of chemisorption, and, critically, the sensing performance of an organic molecule?

Phenytoin Molecule

Nanocages

Metal nanoclusters, such as Gallium (Gan), attract significant attention in nanotechnology due to their semiconducting electronic properties and their potential as nanodetectors or drug carriers. This study focuses on sensing the Phenytoin (Phy) molecule, a compound of pharmaceutical interest.

## Material and Methods

Objectives

- Determine the intrinsic stability and electronic properties of the Ga4 and Ga6 clusters
- Characterize the chemisorption of the Phy molecule on both clusters in the gas phase (adsorption energy Eads)
- Evaluate the sensitivity (ΔEg) and regenerability (recovery time τ) of Ga4 and Ga6 as Phy sensors

### METHOLOGY ( DFT)

Computational Method: Density Functional Theory (DFT)

Functional /Basis Set

B3LYP-D3/6-31G(d,p)

Stability: Binding Energy per atom (Eb) and Fragmentation Energy (ΔEf).

Reactivity: Energy Gap Eg (ELUMO−EHOMO).

Adsorption: Adsorption Energy (Eads) and Gibbs Free Energy (ΔG).

Regenerability: Recovery Time (τ = v −1exp(−Eads/kT)).

Key Calculassions

## Results Discussion

### *1. Stability and Reactivity Results*

**Tableau 1 :** *Stability and Reactivity*

| Cluster | Optimized Geometry | Eg (eV) | Eb (eV/atom) | ΔEf (eV) | Chemical Stability |
|---|---|---|---|---|---|
| **Ga4** | Square (C1) | **0.727** | 1.446 | **0.075** | Low (highly reactive) |
| **Ga6** | Combination of two squares (C1) | **1.689** | 2.015 | **0.120** | High (less reactive) |

Analysis

- Ga4 has the smallest Eg value (0.727 eV) → indicating the highest chemical reactivity
- Ga6 exhibits the largest Eg (1.689 eV) and a peak in fragmentation energy (ΔEf) → Confirming its high chemical stability

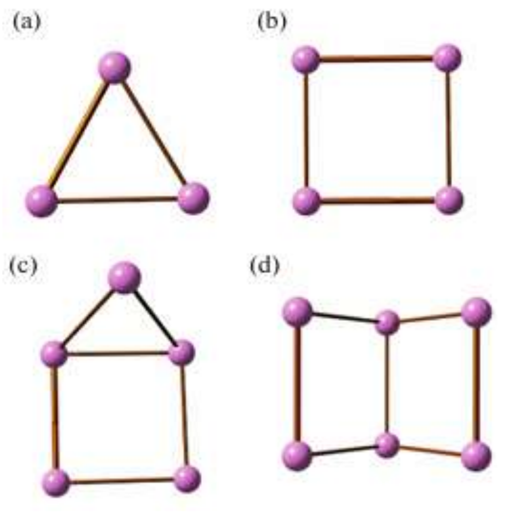
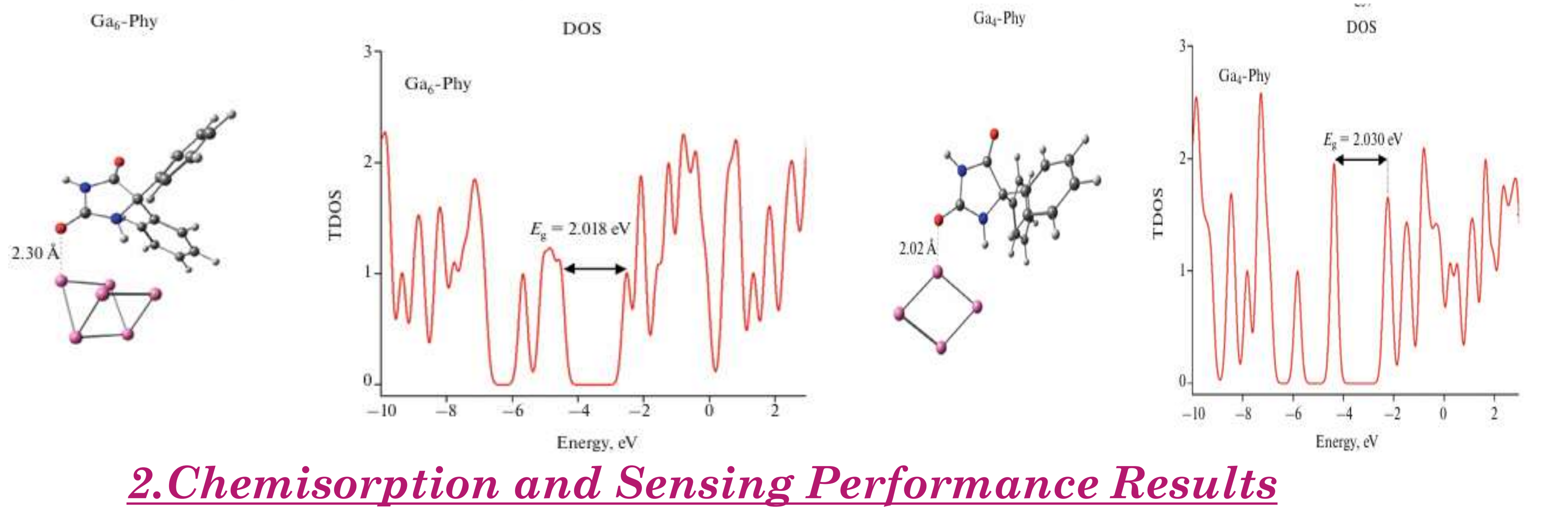



**Fig. 1.** The optimized geometries of the Gan (n = 3–6) clusters.

**Fig. 2.** The optimized geometries and the density of states (DOS) of the Gan-phy complexes




### *2.Chemisorption and Sensing Performance Results*

**Tableau 2 :** Chemisorption and Sensing Performance

| Eads (Gas Phase) | dGa−O (A°) | Eg (After Ads.) | ΔEg (%) | τ (Recovery Time) |
|---|---|---|---|---|
| Phy/Ga4 | -1.566 eV | 2.024 | 2.030 eV | 179.2% |
| Phy/Ga6 | -1.602 eV | 2.297 | 2.018 eV | 19.5% |

Analysis

Adsorption Strength

- Adsorption on both clusters is classified as strong chemisorption (Eads<−1 eV).
- The Phy/Ga6 complex is the most stable (−1.602 eV)

## Results Discussion

Analysis

Sensing Sensitivity

- The dramatic change in Eg for Ga4 (179.2%) upon adsorption suggests very high sensitivity to the Phy molecule
- Ga6 shows much lower sensitivity (19.5%)

Regenerability Limitation

Despite the strong chemisorption, both Ga4 and Ga6 clusters are considered unsuitable for reusable biosensors due to their very long recovery times (τ).

## Conclusion

- ✓ The Ga4 and Ga6 nanoclusters are either **highly reactive** (Ga4) or **highly stable** (Ga6) semiconductors.
- ✓ They exhibit **strong chemisorption** of Phenytoin (Eads≤−1.566 eV).
- ✓ **Ga4** stands out with **exceptional sensitivity** to Phy (179.2% change in Eg).
- ✓ **Limitation:** The long recovery times of Ga4 and Ga6 limit their practical use as reusable sensors, unlike the Ga2 and GaBe11O12 clusters.

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