



3<sup>rd</sup> Korea-US NanoForum, Seoul, Korea, April 3-4, 2006

# Computer-Aided Molecular Design of Nano Bio Sensors

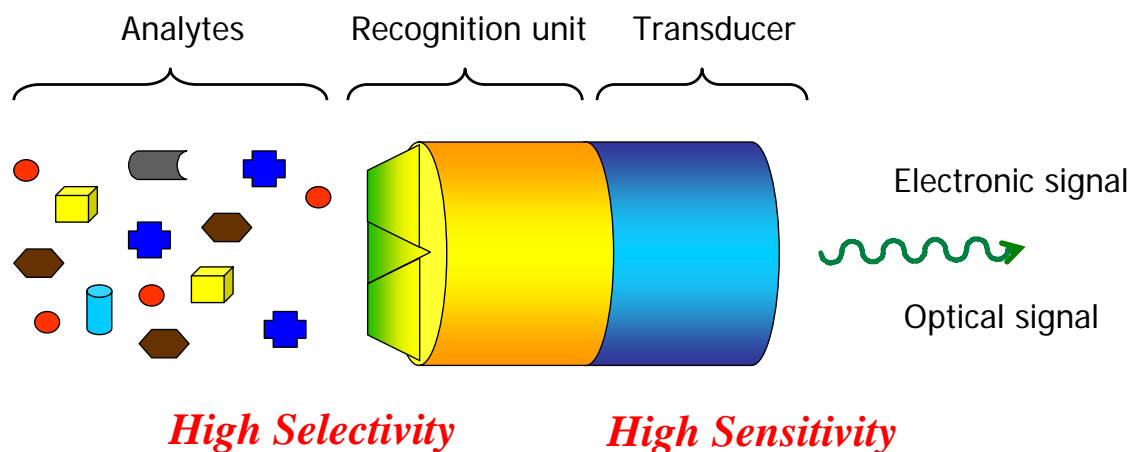
**Sihyun Ham**

*Nano/Bio Computational Chemistry lab.*

Department of Chemistry, Sookmyung Women's University,  
Seoul, Korea



## Nano Bio Sensor



*What is the host?  
What is the guest?  
How they bind?*

- **Structure-Function Relationship**
- **Molecular Recognition**
- **Binding Mechanism**

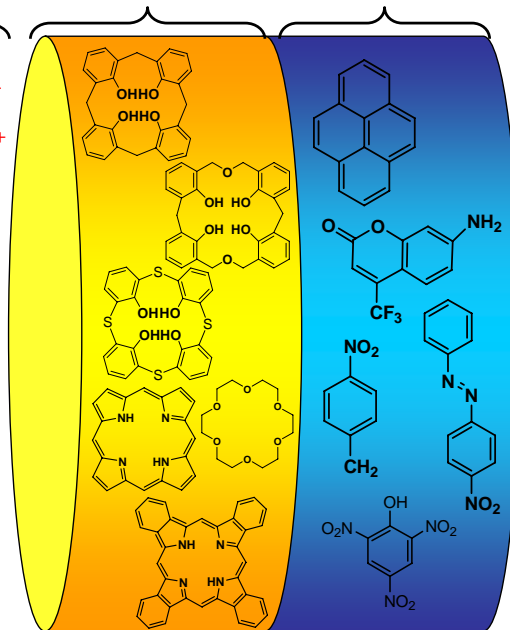


# Nano Bio Sensor

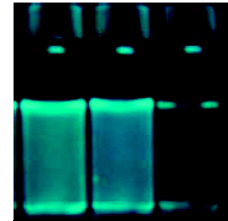
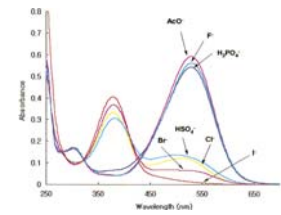
Analytes

$\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\text{Cs}^+$   
 $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Sr}^{2+}$ ,  $\text{Ba}^{2+}$   
 $\text{Ag}^+$ ,  $\text{Zn}^{2+}$ ,  $\text{Pb}^{2+}$ ,  
 $\text{NH}_4^+$ , amine, urea  
 $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  
 $\text{NO}_3^-$ ,  $\text{AcO}^-$ ,  $\text{ClO}_4^-$ ,  
 $\text{H}_2\text{PO}_4^-$ ,  $\text{SO}_4^{2-}$   
amino acid  
Polypeptide  
Protein, DNA  
drugs  
glucose, cholesterol

Recognition unit



Transducer

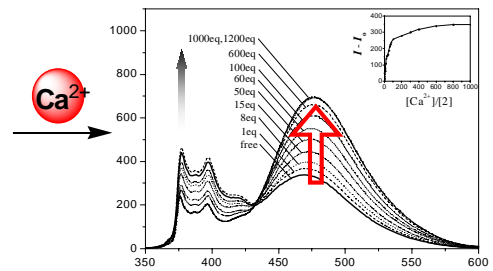
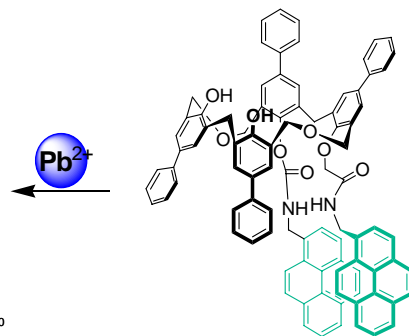
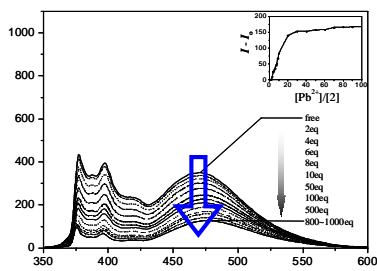


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# Nano Bio Sensor / $\text{Ca}^{2+}$ Sensor

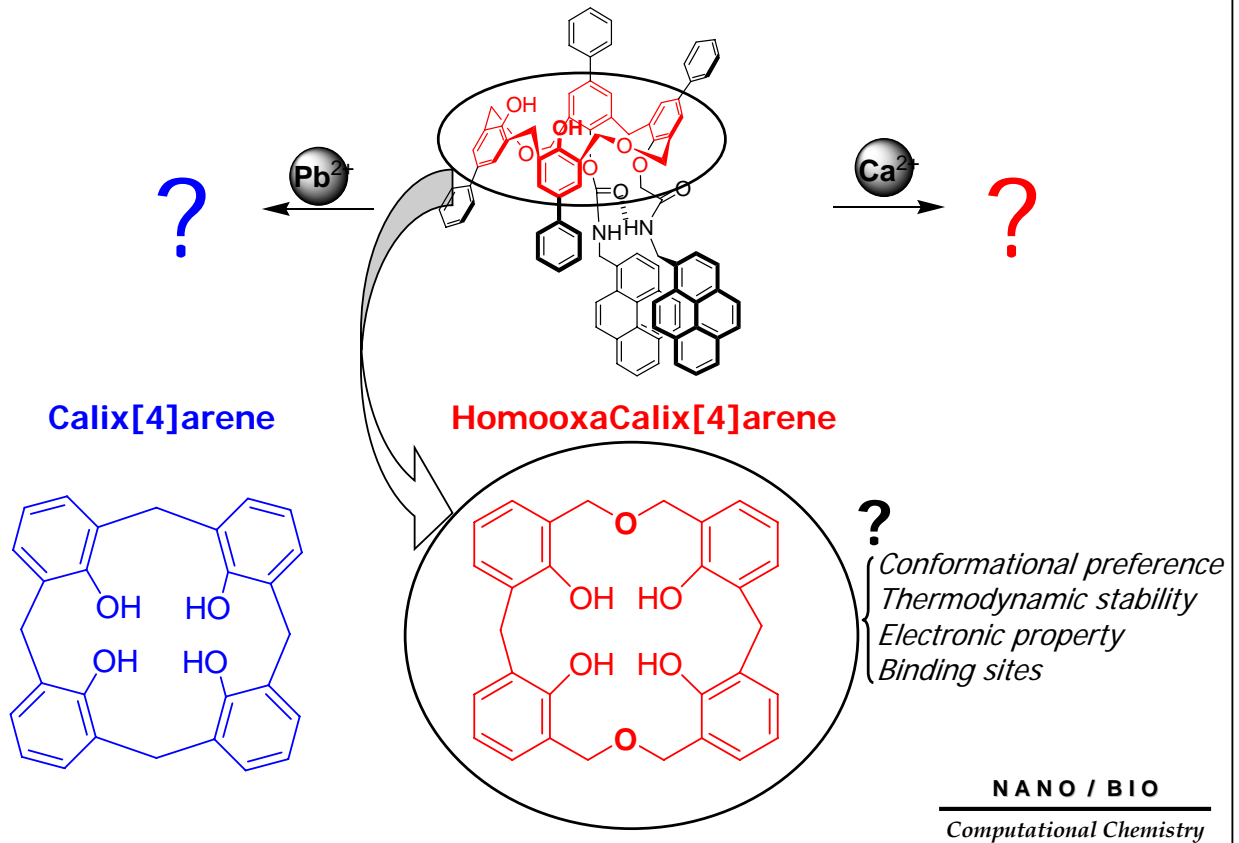


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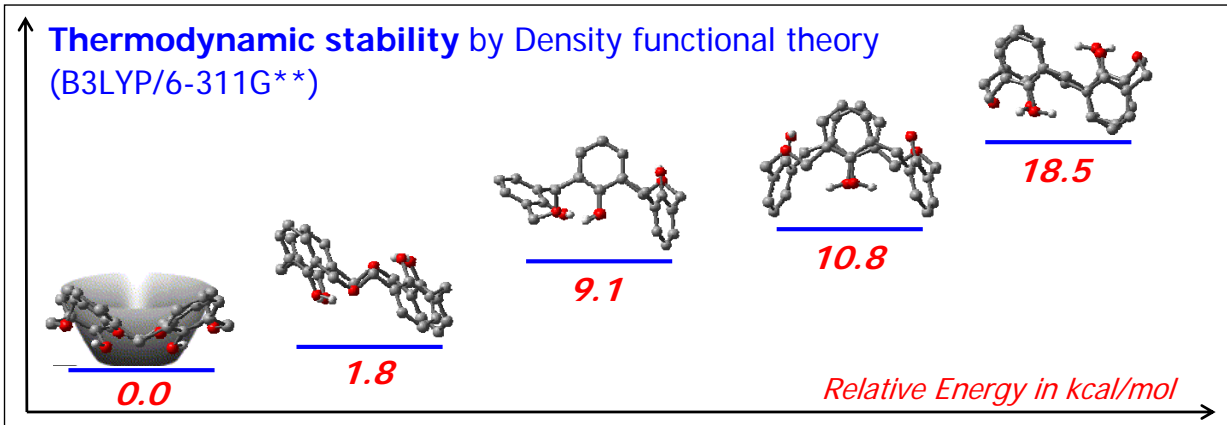
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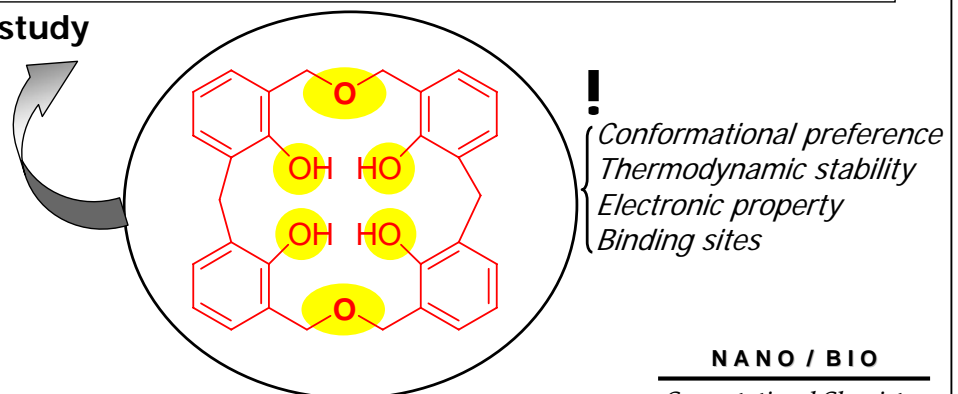
# Nano Bio Sensor / $\text{Ca}^{2+}$ Sensor



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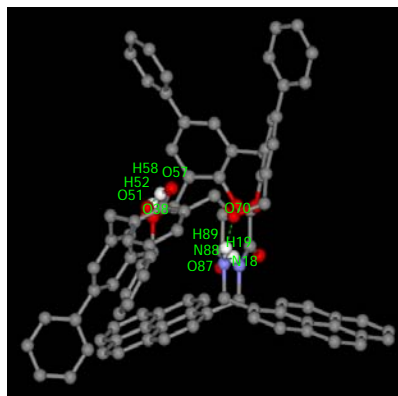
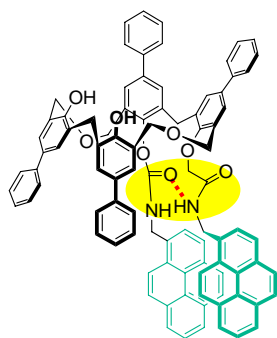


The first theoretical study





## Nano Bio Sensor / $\text{Ca}^{2+}$ Sensor



Hydrogen bonding distance (Å)

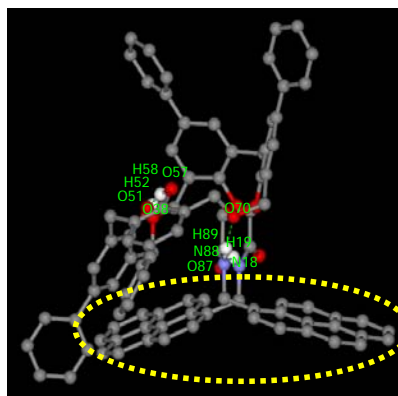
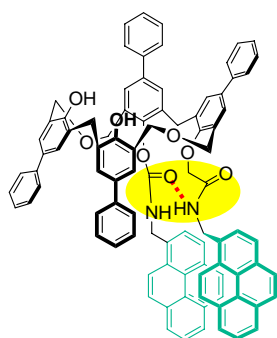
N18-H19...O87	1.89
N88-H89...O70	1.69
O57-H58...O51	1.54
O51-H52...O38	1.51

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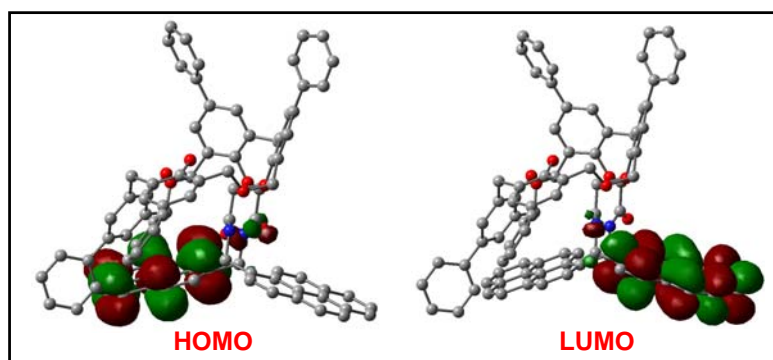


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Py-Py\* interaction -> excimer emission

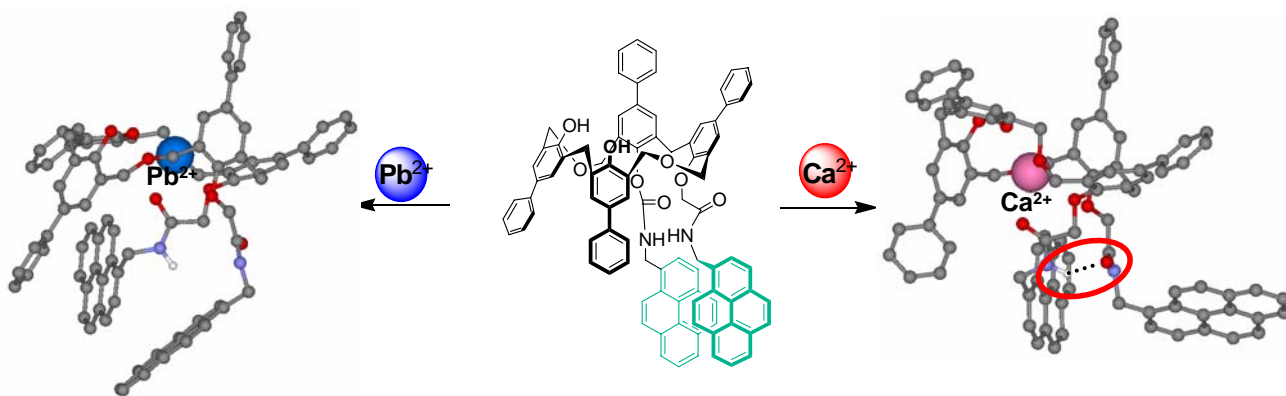
S. Ham, J. Kim et al. *Org. Lett.* **2006**, In Press.

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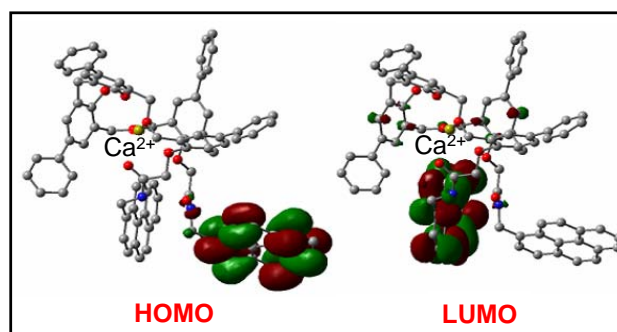
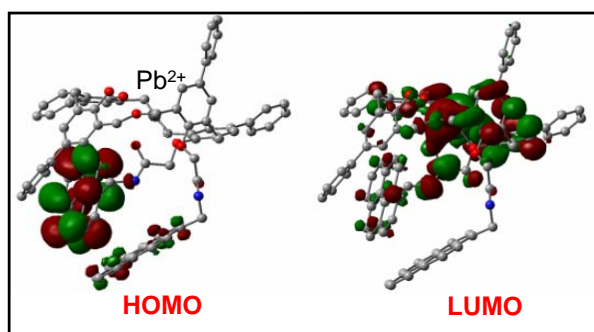


# Nano Bio Sensor / $\text{Ca}^{2+}$ Sensor



$\text{Pb}^{2+}$  complex : Py-Py\* is not observed.

$\text{Ca}^{2+}$  complex : Py-Py\*  $\rightarrow$  excimer emission

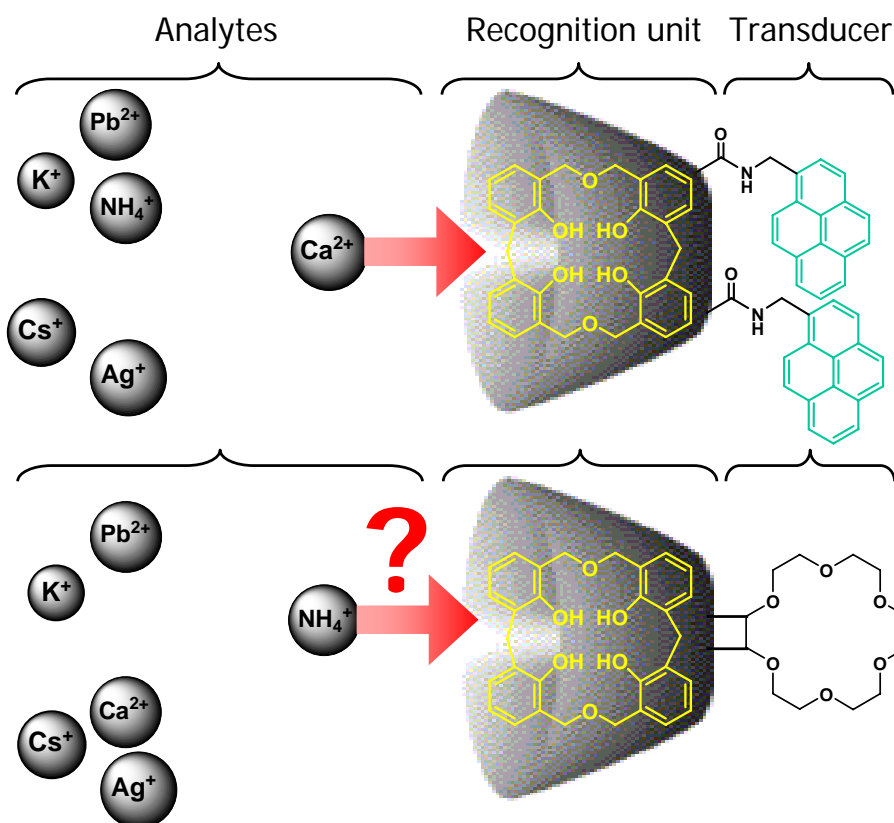


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# Nano Bio Sensor / $\text{NH}_4^+$ Sensor

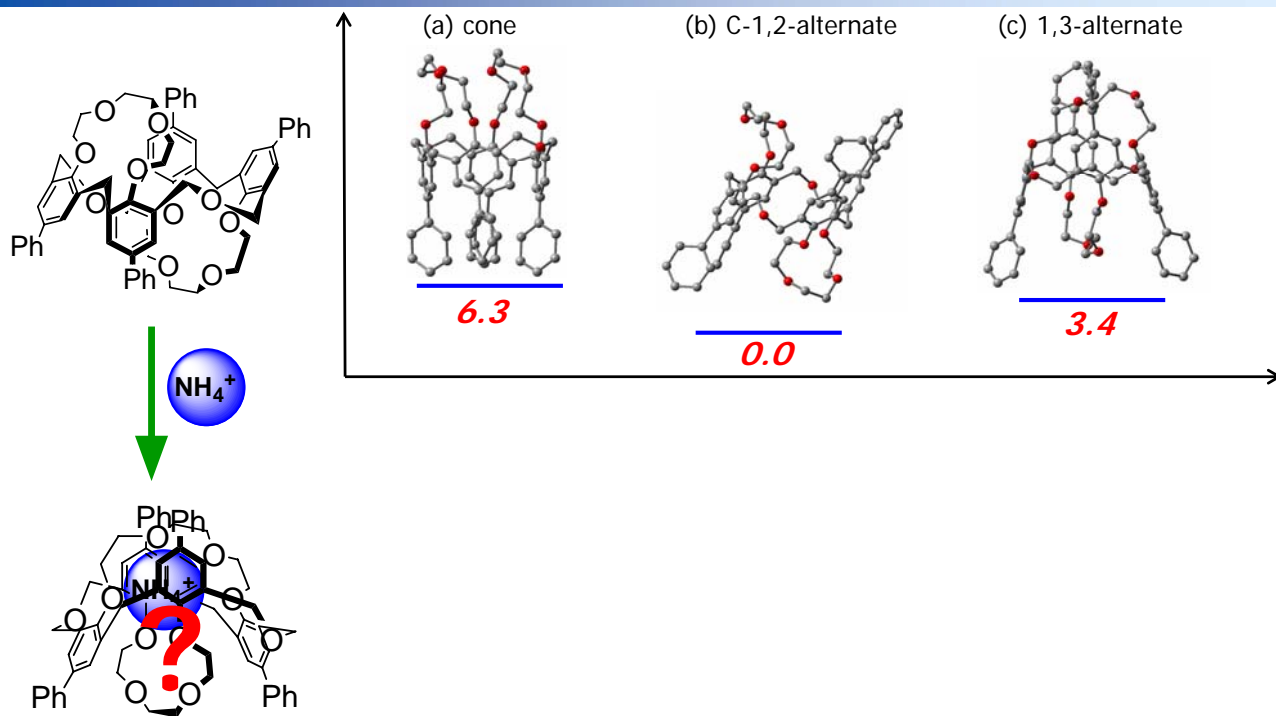


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# Selective Chemical Sensing / $\text{NH}_4^+$ Sensor

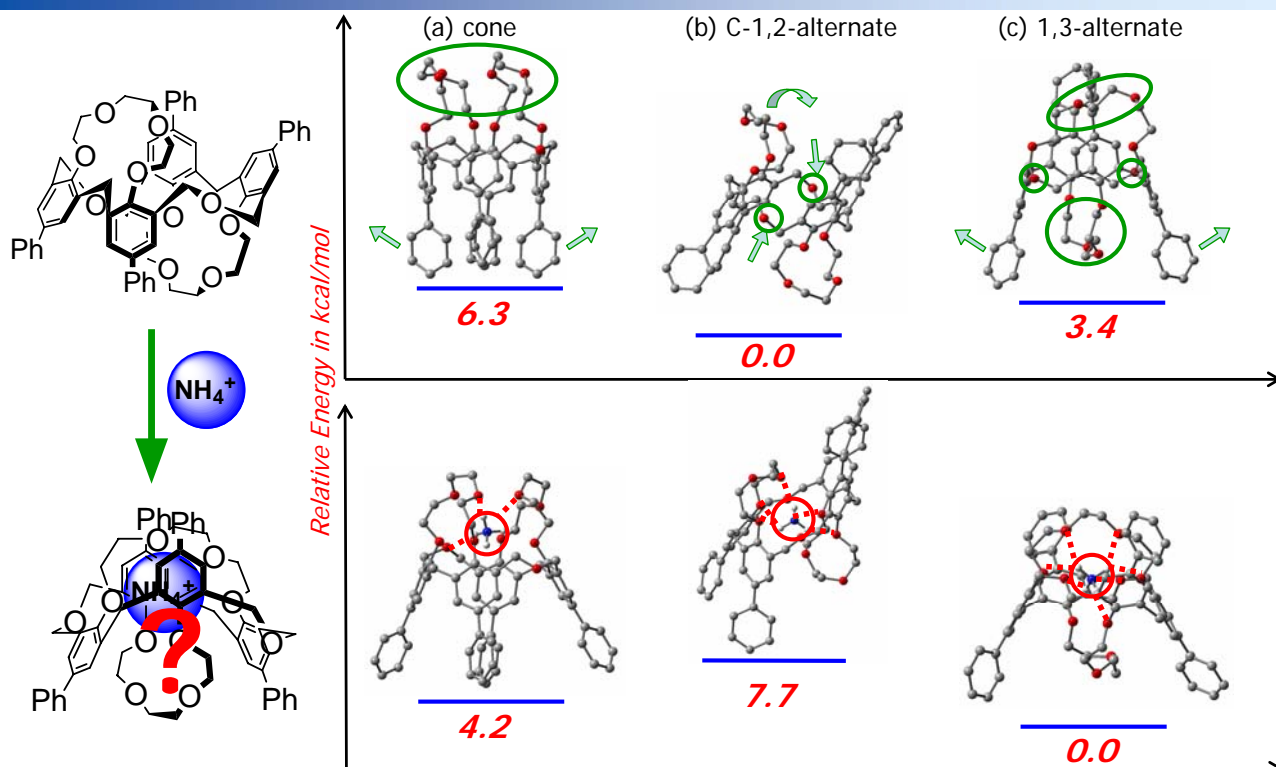


Thermodynamic stability by Density functional theory (B3LYP/6-31G\*)

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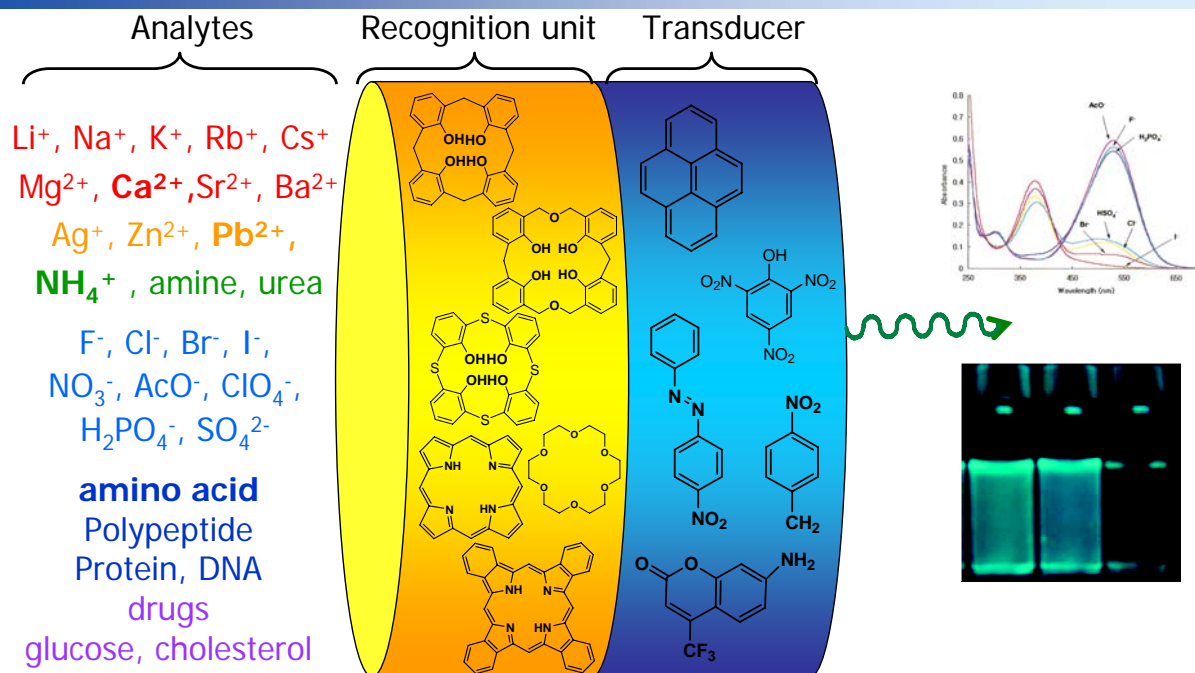


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