

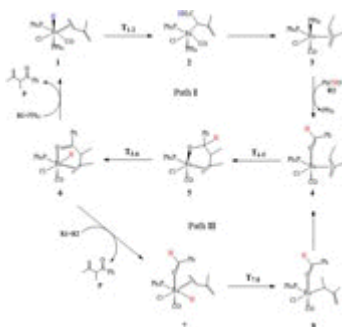
## RESEARCH PAPERS

### 1. Substituent effect and ligand exchange control the reactivity in ruthenium(II)-catalyzed hydroacylation of isoprenes and aldehydes || A DFT study

Qingxi Meng, Peiying Su, Fen Wang, Shuhua Zhu

1650019

A DFT study demonstrated that the ruthenium(II)-catalyzed hydroacylation had two different catalytic cycles (path I and II), and path II was more favorable than path I. The hydroacylation began from the first catalytic cycle. The ligand exchange energy ( $\Delta G_{ex}$ ) had more contribution to the activation barrier than the relative free energy of transition state ( $\Delta G^\ddagger$ ).

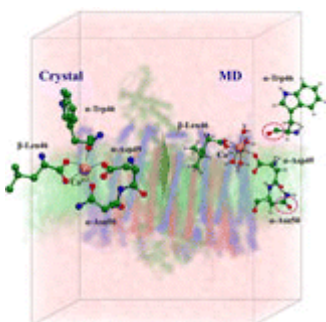


### 2. Computational characterization of the all-atom structure and the calcium binding sites of the LH1-RC core complex from *Thermochromatium tepidum*

M. G. Khrenova, B. L. Grigorenko, J.-P. Zhang, P. Wang, A. V. Nemukhin

1650020

- All-atom model of the bacterial photosynthetic core complex LH1-RC embedded into the membrane is constructed.
- Geometry parameters of the computationally derived model are compared to those of the crystal structure.
- Local structure of the binding sites of the calcium ions at the LH1 subunits is characterized.

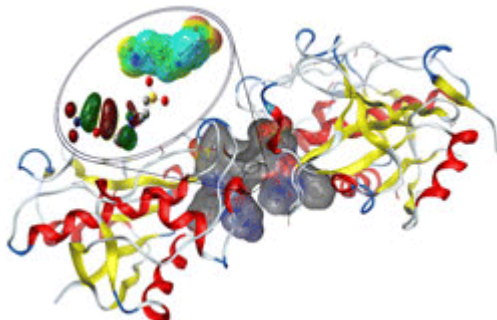


### 3. In silico investigation by conceptual DFT and molecular docking of antitrypanosomal compounds for understanding cruzain inhibition

Toufik Salah, Salah Belaidi, Nadjib Melkemi, Ismail Daoud, Salima Boughdiri

1650021

Current knowledge about Chagas disease, has led to the development of new drugs and the understanding of their mode of action. In this paper, we applied a combination of Conceptual DFT and Molecular Docking for understanding the electronic and steric behaviors of receptorbinding mode of Trypanocidal compounds to guide design and achieving a parasitological cure against Trypanosoma Cruzi. Whereas, a strong agreement with experimental studies was shown.

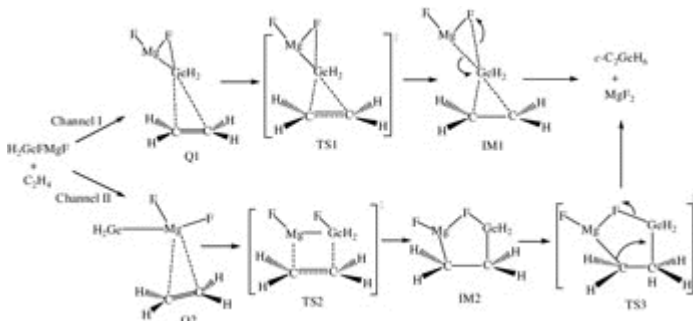


### 4. Theoretical prediction on the addition reaction of germylenoid H<sub>2</sub>GeFMgF with ethylene

Ming-Xia Zhang, Bing-Fei Yan, Wen-Zuo Li, Qing-Zhong Li, Jian-Bo Cheng

1650022

The addition reaction of germylenoid H<sub>2</sub>GeFMgF with ethylene (C<sub>2</sub>H<sub>4</sub>) was firstly investigated using the M062X and QCISD methods. The calculated results demonstrated that there are two different channels in the addition reaction of H<sub>2</sub>GeFMgF with C<sub>2</sub>H<sub>4</sub>, while only the channel I is feasible once the C<sub>2</sub>H<sub>4</sub> approaches H<sub>2</sub>GeFMgF in the proper conditions. The solvent effect on the addition reaction was considered and the results demonstrated that the THF solvent could accelerate the addition reaction.

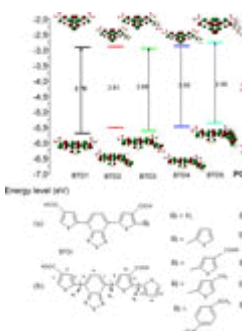


### 5. DFT study of opto-electronic properties of benzothiazole derivatives for use in solar cells

Youssef Ait Aicha, Si Mohamed Bouzzine, Touriya Zair, Mohammed Bouachrine, Mohamed Hamidi, Zakaria Mohyieddine Fahim, Guillermo Salgado Morán, Luis Mendoza-Huizar, Leonor Alvarado-Soto, Rodrigo Ramirez-Tagle

1650023

• Density functional theory used to examine the effect of different electron-donor groups on the structural, electronic and optoelectronic properties of thienylbenzothiadiazole.



• The results suggest that both the introduction of electron-donor groups and the doping process contribute significantly to the electronic and optoelectronic properties of the alternating donor-acceptor-conjugated systems.

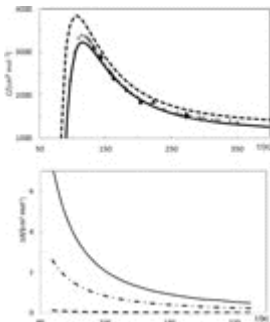
• To provide for the band gap and to guide the synthesis of novel low band gap materials.

## 6. Virial coefficients of nitrogen from a quadrupolar site–site potential function

Kenneth Osondu Monago, Charles Otoberise

1650024

A method for the numerical calculation of third volumetric and acoustic virial coefficients of symmetric linear molecules was applied to nitrogen using a site–site model potential function. The contributions of quadrupole-quadrupole interactions to the virial coefficients were investigated. The results suggest that, on certain isotherms, the contributions to the second and third virial coefficients exceeded twenty percent.

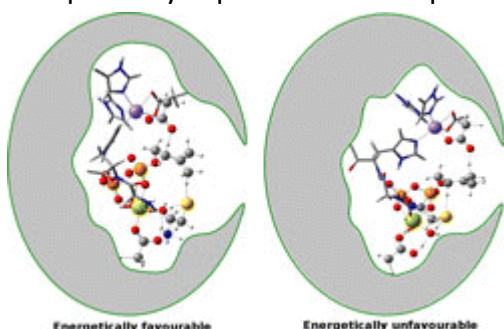


## 7. DFT study on the mechanism of 1,3-hydrogen disposition in Isopentenyl pyrophosphate catalyzed by Isopentenyl pyrophosphate: Dimethylallyl pyrophosphate isomerase

Atanu Basak, Kuheli Chakrabarty, Animesh Ghosh, Gourab Kanti Das

1650025

Isomerization reaction catalysed by IPP-DMAPP isomerase was previously considered to take place through the formation of carbocation intermediate. Our theoretical study on the pathway of this isomerization reaction at the active site of the enzyme suggests a concerted mechanism that occurs through a single transition state without generating any carbocation intermediate. This pathway explains several experimental observations previously reported in literature.

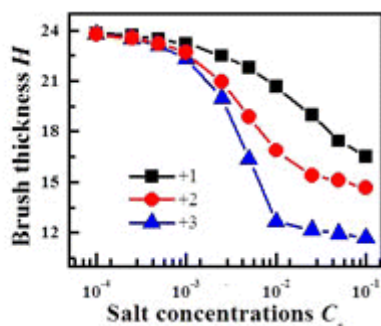
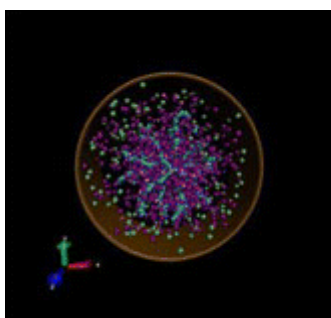


## 8. Molecular dynamics simulations of cylindrical polyelectrolyte brushes in monovalent and multivalent salt solutions

Qing-Hai Hao, Qian Chen, Zhen Zheng, Li-Yan Liu, Tie-Ju Liu, Xiao-Hui Niu, Qing-Gong Song, Hong-Ge Tan

1650026

- The collapse of brush is observed with increasing salt concentration.
- The non-uniform stretching structure of the chains is characterized.
- The ion-exchange effect on the shrink of brushes is illustrated.



## 9. Theoretical investigations on charge transfer properties of fluorinated perylene diimides

Meng Liang, Jun Yin, Kadali Chaitanya, Xue-Hai Ju

1650027

The charge transfer properties of perylene diimide (PDI) and its fluorinated derivatives have been investigated by density functional theory (DFT) coupled with the incoherent charge-hopping model. The p-type organic semiconductor of PDI could be converted to *n*-type or ambipolar ones (DF-PDI and TF-PDI) by attaching a moderate number of electron-withdrawing fluorines to the bay region. The maximal charge mobilities occur in direction of the parallel  $\pi$ - $\pi$ stacking dimers.

