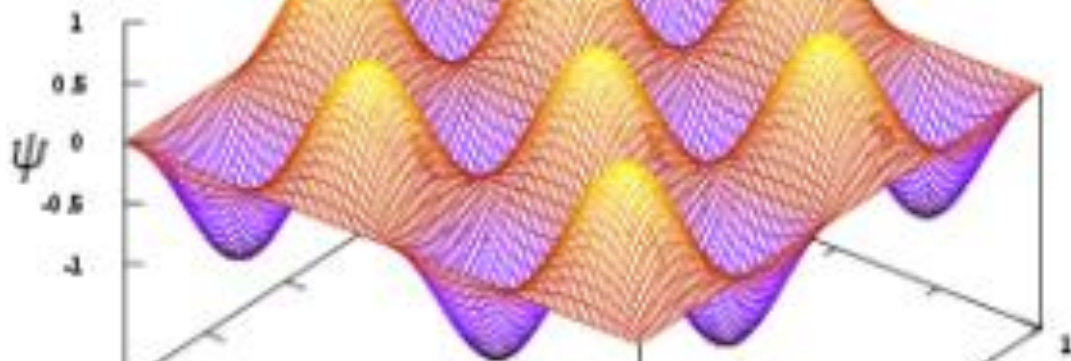


# Faculty of Sciences - School of Chemistry



## Laboratory of Quantum and Computational Chemistry

November 2023

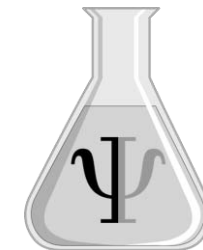


**Aristotle University of Thessaloniki - Faculty of Sciences**

## **School of Chemistry**

# **Laboratory of Quantum and Computational Chemistry**

## **Teaching – Research Fields - People**



### **Teaching**

Quantum Chemistry  
Computational Chemistry  
Molecular Modelling  
Molecular Symmetry  
Mathematics  
Information and Communication  
Technologies (ICT) in Chemistry  
Education

### **Research**

Quantum Chemistry  
Molecular Mechanics  
Molecular Dynamics  
Machine Learning  
Information and  
Communication Technologies  
(ICT) in Chemistry Education

### **2018 – 2023: Five Years of Growth**

**2018**

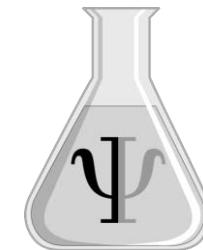
**2 Members**

**2 Papers/Year**

**2023**

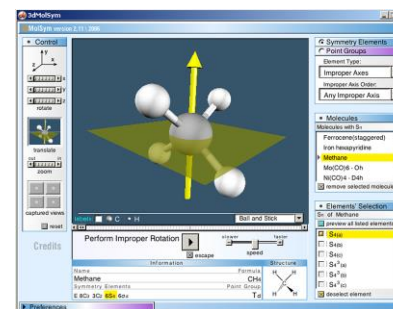
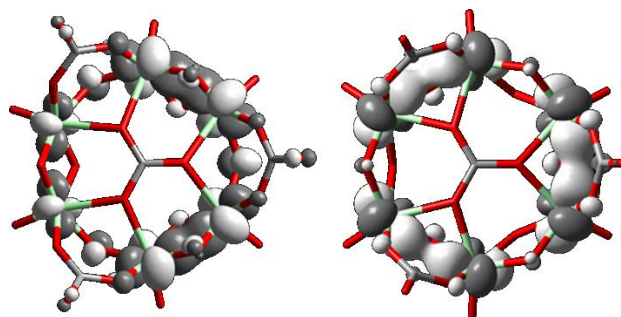
**5 Members**

**11 Papers/Year**

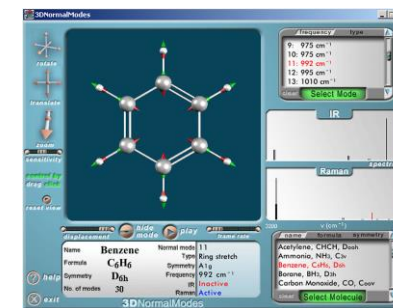
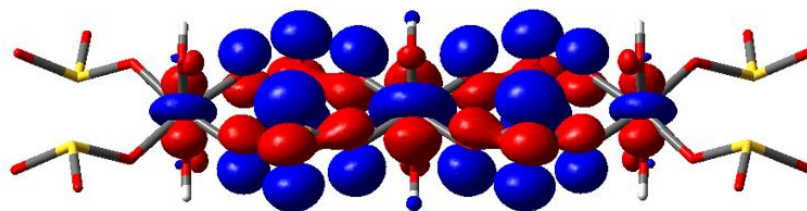


Research

- Quantum chemical study of bonding and properties of transition metal complexes
- Electronic structure, bonding, magnetic properties and molecular interactions
- Development of educational software and web content for Chemistry education



CHEM  
NOESIS



Michael P. Sigalas

Professor

Current Director

Teaching

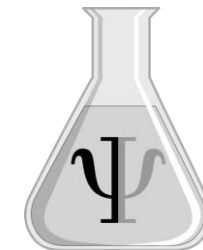
Quantum Chemistry

Computational Chemistry

Molecular Symmetry

Mathematics

ICT in Chemistry Education



### Research

- Mechanical, elastic, vibrational properties and spectroscopy of graphene
- Design of materials for gas storage
- Design of molecular structures (small molecules and polymers) for organic solar cells

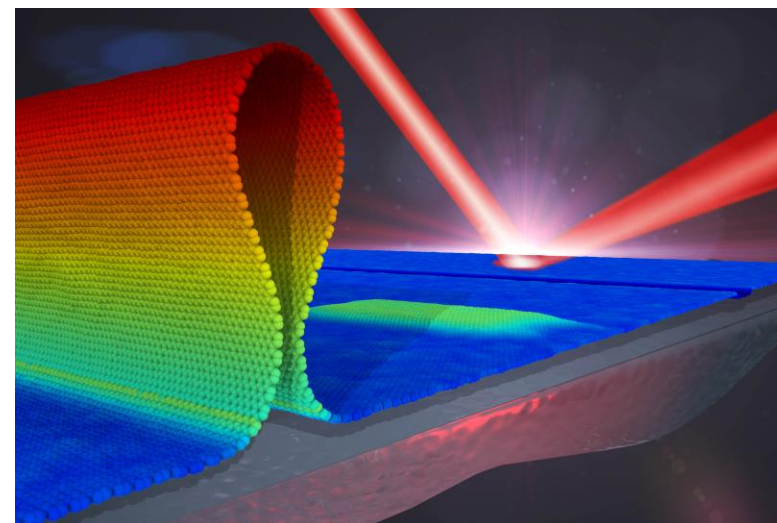
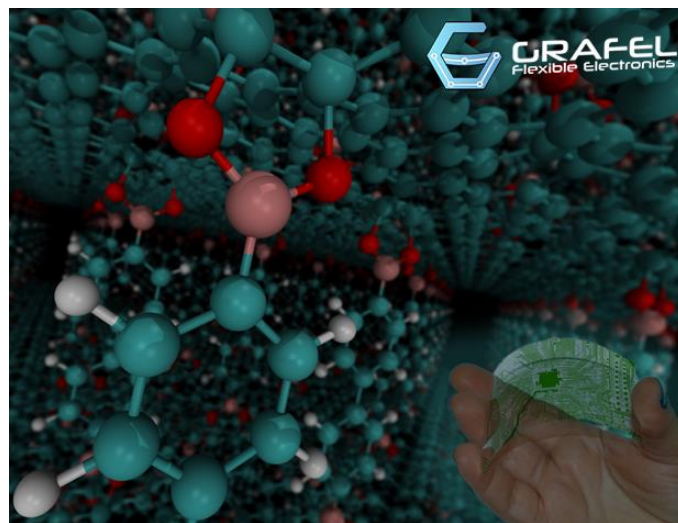


**Emmanuel Koukaras**

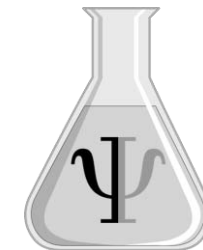
Assistant Professor

### Teaching

Quantum Chemistry  
Computational Chemistry  
Mathematics

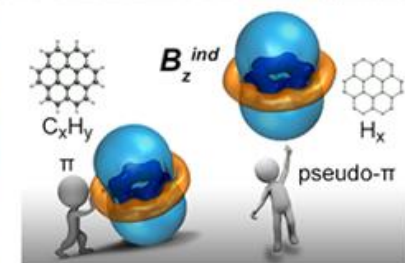
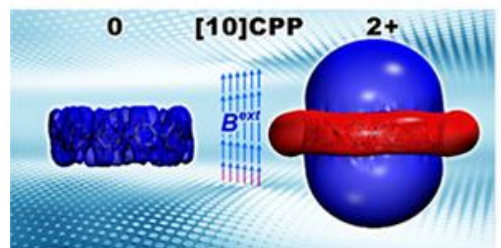
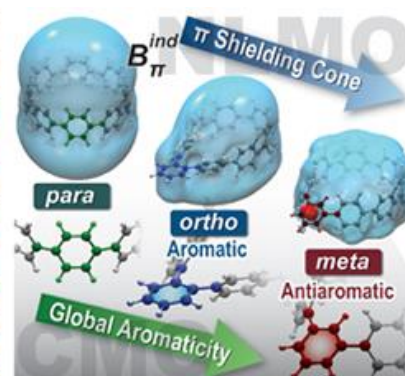




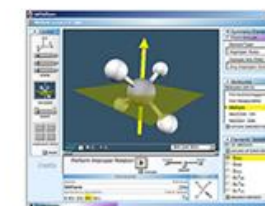
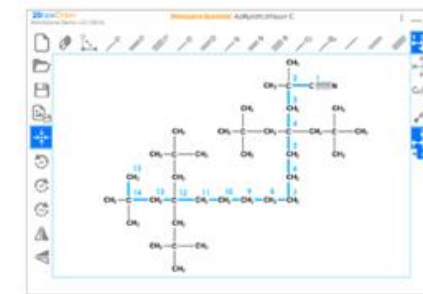


### Research

- *Aromaticity research:* Magnetic response.  $\pi$ -Conjugated molecules. Polycyclic Aromatic Hydrocarbons. Nanocarbons. Nano hoops. Supramolecular aromatics.
- *Educational Chemistry:* Multirepresentational media for Chemical Education. Cognitive tools and Visuospatial thinking in Chemistry learning.



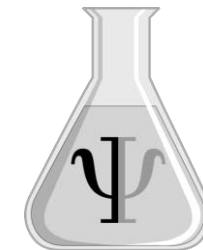
CHEM  
NOESIS



**Nikolaos Charistos**  
Assistant Professor

### Teaching

Computational Chemistry  
Mathematics  
ICT in Chemistry Education



**Georgios Fanourgakis**  
Assistant Professor

### Research

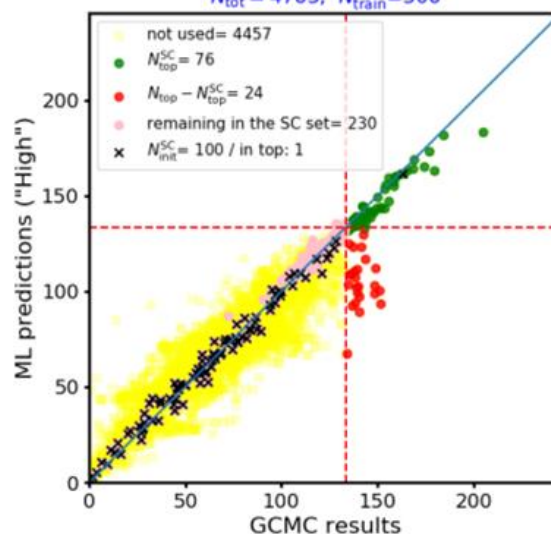
- Development of force fields for intermolecular interactions from ab initio electronic structure calculations
- Study of water and aqueous solutions by classical and quantum Molecular Dynamics simulations.
- Application of Machine learning techniques in physical chemistry related problems.

#### Self Consistent Machine Learning Algorithm

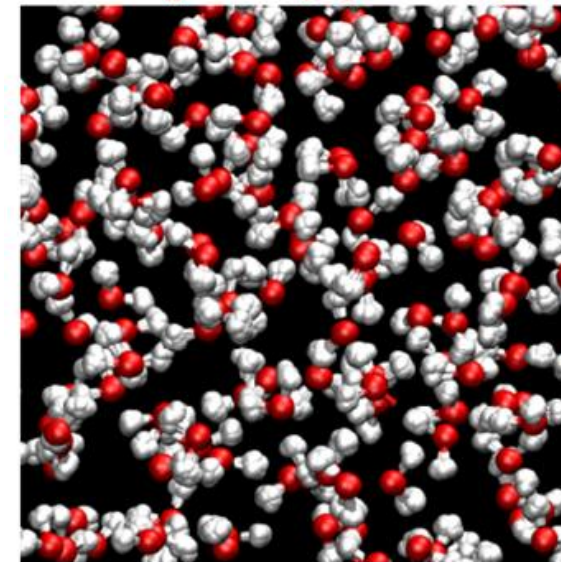


CH<sub>4</sub> (CoRE MOFs), T = 298 K, P = 5.8 bar

$N_{tot} = 4763$ ,  $N_{train}^{SC} = 306$

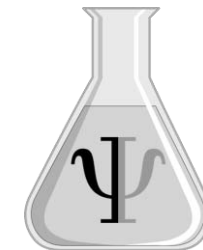


#### Path Integral MD (liquid water)



**Teaching**  
Computational Chemistry  
Molecular Modelling  
Mathematics





Research

- Exploration of the understanding of multiple representations in chemistry education with eye tracking methodology.
- Development of Web Applications and Multimedia Learning Environments for Science Education and Research.



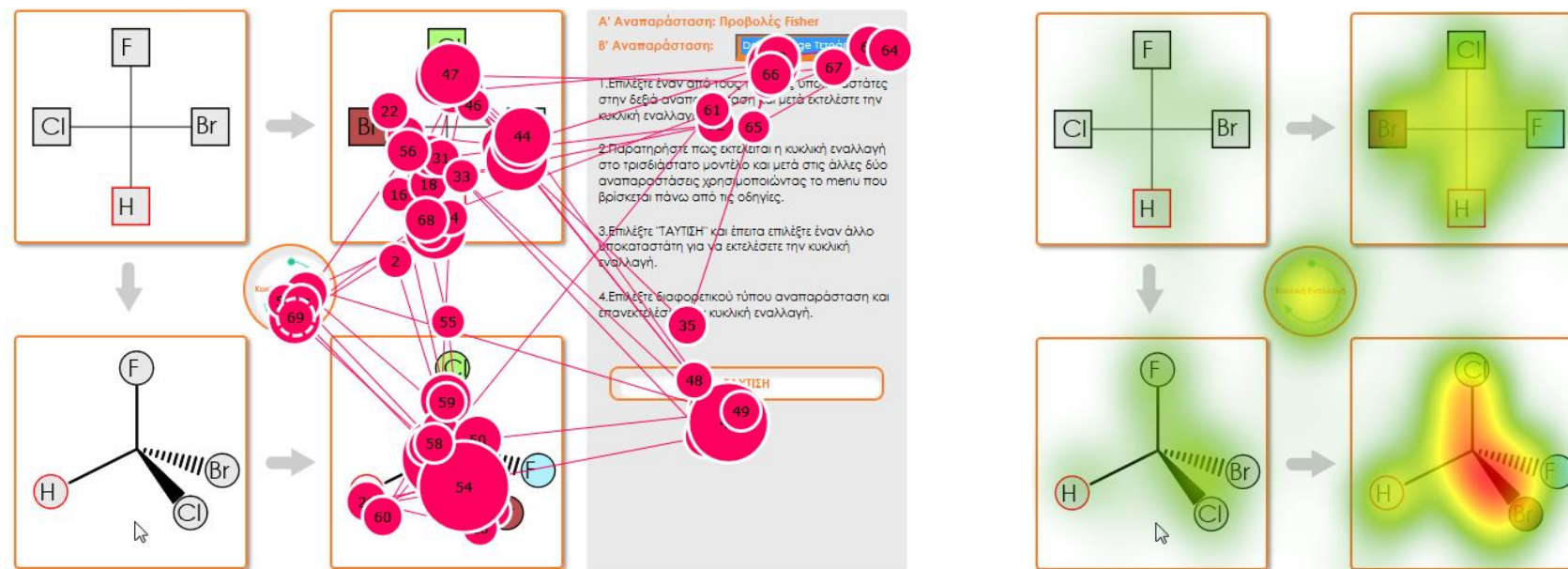
Vasilios Koutalas

PhD

Laboratory Teaching Staff

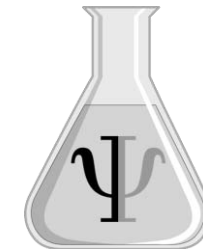
Teaching

Computational Chemistry  
ICT in Chemistry Education



## School of Chemistry

# Laboratory of Quantum and Computational Chemistry Infrastructure



### Hardware

- Laboratory's Computer Cluster with a total of 180 cores and 1.2 TB RAM, interconnected with 10 GbE.
- Laboratory's 8 Workstations
- Access to Institutional HPC facilities (partition) with 3100 CPU cores and 10 TB RAM, interconnected via 200G InfiniBand

### Software

#### • *Commercial*

- Gaussian 16
- GaussView 6
- Turbomole 7.7
- Crystal 2017
- WebMO Enterprise 2022
- Amsterdam Modeling Suite (ADF) 2020
- NBO 7

#### • *Open Source*

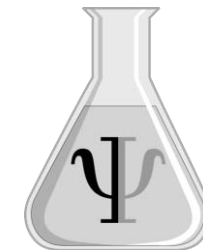
- ORCA
- CP2K
- Quantum Espresso
- CASTEP
- NWChem
- LAMMPS
- GROMACS
- NAMD
- Tinker





## School of Chemistry

# Laboratory of Quantum and Computational Chemistry Collaborations - Students



### Collaborations with Other Institutions

- Facultad de Ingeniería, Arquitectura y Diseño, Universidad San Sebastián, Santiago, Chile.
- LNM Institute of Information Technology, India.
- Pacific Northwest National laboratory, Washington State, United States.
- University of Oxford, Chemistry Department, United Kingdom.
- Institute of Analytical Sciences and Physico-Chemistry for Environment and Materials (IPREM ) @ Pau/CNRS/UPPA, France.
- Chemical Engineering Department, Abu Dhabi University, United Arab Emirates.
- Chemical Engineering Department, Khalifa University, United Arab Emirates.
- Composites and Nanomaterials Laboratory (CNML) @ FORTH/ICE-HT, Greece.
- Inorganic Chemistry Laboratory, Chemistry Department, Aristotle University Of Thessaloniki, Greece.
- Food Chemistry and Technology Laboratory, Chemistry Department, Aristotle University Of Thessaloniki, Greece.
- University of Crete, Chemistry Department, Physical Chemistry Laboratory, Greece.
- Division of Chemistry, Chemical Engineering Department, Aristotle University Of Thessaloniki, Greece.
- Center for the Dissemination of Science and Technology Museum. Noesis, Greece.

### Current Students

- *16 Undergraduate students working on Diploma Thesis*
- *8 Graduate students working on Ms Thesis*
- *4 PhD students working on PhD Thesis*

