

## CURRICULUM VITAE

### Anastasios Papadopoulos

Post-Doctoral Researcher  
Theoretical and Physical Chemistry Institute  
National Hellenic Research Foundation  
48 Vassileos Constantinou Ave.  
Athens 11635, Greece

Phone: +30 210 7273813

Fax: +30 210 7273794

E-mail: [anastp@eie.gr](mailto:anastp@eie.gr)



---

### EDUCATION

- Ph.D. in Computational Chemistry, School of Physical Sciences, Chemistry Department, Aristotle University of Thessaloniki, Greece (2012)
- M.Sc. in Physical Chemistry and Electrochemistry, School of Physical Sciences, Chemistry Department, Aristotle University of Thessaloniki, Greece (2013)
- M.Sc. in Applied Quantum and Computational Chemistry, School of Physical Sciences, Chemistry Department, Aristotle University of Thessaloniki, Greece (2006)
- B.Sc. in Chemistry, School of Physical Sciences, Chemistry Department, Aristotle University of Thessaloniki, Greece (2004)

### PROFESSIONAL EXPERIENCE AND APPOINTMENTS

09/2018 – present: Post-Doctoral Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Greece

02/2017 – 08/2017: Scholar Lecturer in Computational Chemistry, Laboratory of Applied Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Greece

09/2016 – 09/2017: Post-Doctoral Researcher, Laboratory of Applied Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Greece

11/2012 – 12/2015: Researcher Chemist, Laboratory of Applied Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Greece

### **MAIN RESEARCH INTERESTS**

- Molecular Electronic Structure Theory of amorphous inorganic systems
- Structural, Electronic and Magnetic properties of aromatic compounds
- TD-DFT and Spectroscopic properties on metal complexes
- Long-range interactions in polymers
- Antioxidant activity of organic compounds using computational methods

### **TEACHING EXPERIENCE**

- Scholar Lecturer in Computational Chemistry, Laboratory of Applied Quantum and Computational Chemistry, Aristotle University of Thessaloniki, Greece

### **EXTERNAL FUNDING**

- IKY Fellowships of Excellence for Postgraduate Studies in Greece – Siemens Program, 2016-2017.
- Education and Lifelong Learning of the National Strategic Reference Framework (NSRF)-Research Funding Program: Thales, 2012-2015.
- Theoretically study of polymeric mixtures as bodies release in pharmaceutical compounds, Research Funding Program by Pharmathen S. A. company.

### **PROFESSIONAL AFFILIATIONS & ACTIVITIES**

- Reviewer for the journals *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (Elsevier), *Journal of Computational and Theoretical Chemistry* (Elsevier).

### **CONFERENCES**

- “*Visualization of the molecular orbitals contribution to the induced magnetic field of heterocyclic isocoronene analogues.*” Conference on Current Trends in Computational Chemistry, 10 - 11 November 2017, Jackson, Mississippi, USA.

- "Visualization of Substituents' Effects on  $n$  Electron Delocalization in B-Trisubstituted Borazines" World Association of Theoretical and Computational Chemists (WATOC), 5–10 October 2014, Santiago, Chile.
- "Molecular Orbital Contributions to the Induced Magnetic Field of Benzene, Cyclobutadiene, Borazine, 1,2-, 1,3-, and 1,4-Azaborines." World Association of Theoretical and Computational Chemists (WATOC), 17–22 July 2011, Santiago de Compostella, Spain.

## SELECTED PUBLICATIONS

1. V. Styliou, K. Kavaratzi, I. Papazoglou, A. G. Hatzidimitriou, A. G. Papadopoulos, P. Angaridis, and P. Aslanidis (**2018**) "Binuclear Copper(I) Compounds with N-Heterocyclic Thiolate and Diphosphane Ligands: Effects of Thiolate Ligands on Solid- State Molecular Structures and Luminescence Properties." *Eur. J. Inorg. Chem.*, **2018**, 2915-2926.
2. N. D. Charistos, A. G. Papadopoulos, T. A. Nikopoulos, A. Muñoz-Castro and M. P. Sigalas (**2017**) "Canonical Orbital Contributions to the Magnetic Fields Induced by Global and Local Diatropic and Paratropic Ring Currents." *Journal of Comput. Chem.*, **38**, 2594-2604.
3. A. G. Papadopoulos, N. D. Charistos and A. Muñoz-Castro (**2017**) "Magnetic Response of Aromatic Rings Under Rotation. Aromatic Shielding Cone of Benzene Upon Different Orientations of the Magnetic Field." *ChemPhysChem.*, **18**, 1499-1502.
4. A. G. Papadopoulos, N. D. Charistos, K. Kyriakidou and M. P. Sigalas (**2015**) "Study of Electron Delocalization in 1,2-, 1,3- and 1,4-Azaborines based on the Canonical Molecular Orbital contributions to the Induced Magnetic Field and Polyelectron Population Analysis." *J. Phys. Chem. A*, **119**, 10091-10100.
5. E. Karavas, E. Koutris, A. G. Papadopoulos, M. P. Sigalas, S. Nanaki, G. Z. Papageorgiou, D. Z. Achilias, D. N. Bikiaris, (**2014**) "Application of density functional theory in combination with FTIR and DSC to characterise polymer drug interactions for the preparation of sustained release formulations between fluvastatin and carrageenans." *International Journal of Pharmaceutics*, **466**, 211–222.
6. I. Papazoglou, P.J. Cox, A.G. Papadopoulos, M.P. Sigalas, and P. Aslanidis (**2013**) "Copper (I) complexes of 1,10-phenanthroline and heterocyclic thioamides: An experimental and theoretical (DFT) investigation of the photophysical characteristics." *Dalton Trans.*, **42**, 2755 –2764.