

## CV

### Demeter Tzeli

Associate Professor of Chemistry



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Marital status: married with 5 children

#### • Education and Seminars

7/1995: B.S. in Chemistry, Department of Chemistry, National and Kapodistrian University of Athens (NKUA), Greece.  
10/1997: M.Sc. in Physical Chemistry, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece.  
7/1998: Summer School, Cornell University, Ithaca, N.Y., USA  
7-9/1998: Pacific Northwest National Laboratory, Richland, U.S.A (PhD fellow)  
11/2000: Ph.D. in Quantum Chemistry, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece.  
11/2014: PRACE Autumn School in HPC Programming Techniques, Center of the Hellenic Telecommunications Organization (OTE Academy), Athens, Greece.

#### • Work Experience

12/2000-8/2006: Post-doctoral Researcher, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece.  
12/2001-10/2002: Teacher of computer science in private college, KORELplus, 85 Akadimias, 10678 Athens, Greece.  
10-11/2004: Visiting Researcher, Theoretical Chemistry, Materials Science Center, Rijksuniversiteit Groningen, the Netherlands, HPC-Europa Transnational Access programme  
9/2006-3/2013: Post-doctoral Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece.  
3/2013-7/2014: Post-doctoral Researcher, Institute of Nanoscience and Nanotechnology, Demokritos, National Center of Scientific Research, Agia Paraskevi Attikis, P.O. Box 60228, Athens 15310, Greece.  
8/2014-7/2018: Post-doctoral Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece.  
8/2018- : Collaborating Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece.  
9/2019-4/2020: Visiting Professor, Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 157 71, Greece  
5/2020: Associate Professor "Physical Chemistry – Theoretical Molecular Quantum Chemistry".

#### • Honors and Awards

- Undergraduate:
  - Scholarship of Women Association of Trikala (for achieving the highest score at the entrance examinations for the Chemistry Department) (1991-1995).
  - National Scholarship Foundation of Greece (for academic achievement) (1991-1995)

2. Graduate:
  - National Scholarship Foundation of Greece (11/1996-4/2000)
  - Associated Western Universities (AWU), USA, Laboratory Graduate Fellowship (7-9/1998)
3. Post-doctoral:
  - Fellowship of Academy of Athens (9/2002-6/2004)
  - HPC- Europa Transnational Access programme (10-11/2004) (Researcher)
  - FP7-Capacities-Research Potential Of Convergence Regions (5/2008-1/2011) (Research Associate)
4. Awards:
  - Greek Award 2009 L'ORÉAL-UNESCO for the Women in Science.

• **National, European and International Projects**

1. AWU program (7-9/1998)  
 “Studying the acetylene-water interaction,  $C_2H_2-(H_2O)_n$ ,  $n = 1 - 4$ .”  
 PhD fellow, Pacific Northwest National Laboratory, Richland, U.S.A.
2. SSATES, EPEAEK (5/1999-12/1999)  
 “Design and operation of station for continued upgrading of technological studies”  
 Teaching computer usage to undergraduate chemistry students at NKUA.
3. Pythagoras, EPEAEK II (7/2004-8/2006)  
 This project is co-funded by the European Social Fund and National Resources.  
 “Accurate ab initio calculations on the  $MC_x^{0,\pm 1}$ ,  $MB_x^{0,\pm 1}$   $M_y$  molecules,  $M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni$  and  $Cu$ ,  $x = 1, 2$ ,  $y = 2, 3$ .”  
 Researcher, Lab. Physical Chemistry, Department of Chemistry, NKUA, Greece.
4. HPC- Europa Transnational Access programme (10-11/2004)  
 “Analysis of the chemical bonding of the superconductor  $MgB_2$ .”  
 Research Associate Visitor, Theoretical Chemistry, Materials Science Center, Rijksuniversiteit Groningen, the Netherlands.
5. Greek-Slovakian collaboration (9/2006-4/2008)  
 “Theoretical calculations on clusters of GaN and InN molecules and their interaction with Si(111) surface.”  
 Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vassileos Constantinou 48, Athens
6. Visiting scientist to the Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University, Mlynská dolina, Bratislava, Slovakia, (Prof. M. Urban), 24-30/6/2007.
7. FP7-Capacities-Research Potential Of Convergence Regions (5/2008 – 12/2011)  
 “Carbon Nanohorn-based Hybrid Materials for Energy Conversion. Reinforcing and Expanding the Research Potential of Carbon-Nanostructures Laboratory to a Regional and European Kernel of Excellence”  
 Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
8. NATO Science For Peace And Security Programme (7/2009 – 7/2011)  
 “Fluorescent sensors for organophosphorous nerve agent mimics and other warfare agents”  
 Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
9. Visiting scientist to the Department of Theoretical Chemistry, Bergische University GH Wuppertal, Germany (Prof. Dr. R. J. Buenker) (6/2010)
10. *COMANA* “ARISTEIA” (3/2013 – 7/2014)  
 “Complex Magnetic Nanostructures”  
 Research Associate, Institute of Nanoscience and Nanotechnology, Demokritos, National Center of Scientific Research, Agia Paraskevi Attikis, P.O. Box 60228, Athens 153 10, Greece
11. *POLINANO*, *KRIPIS*, *ESPA* (8/2014 – 12/2015)  
 “New Multifunctional Nanomaterials και Devices”  
 Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens

12. Visiting scientist to the Physics Department of the Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Lisbon, Portugal (4/2017) (STSM grant)  
“Study of the interaction of catechin molecules with lipids”
13. Competitiveness, Entrepreneurship and Innovation, NSRF(2014-2020), (12/2017-12/2018)  
“Advanced Materials and Devices”  
Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
14. 12<sup>th</sup> Cy-Tera and Eastern Mediterranean production access resource allocation, HPC resource of Bibliotheca Alexandrina, (12/2017-12/2018)  
"Interaction of catechins with phospholipids"  
Project leader, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
15. PNNL and TPCI/NHRF project (Coordinator), contract: 400432 (3/2018-6/2019)  
"Electronic states of single and multiple metal centers in systems of catalytic and biological importance."  
Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
16. PNNL and Chemistry Department/NKUA project (Coordinator), contract: 493175/15810 (29/10/2019-30/06/2020) "Electronic states of single and multiple metal centers in systems of catalytic and biological importance." Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Panepistimiopolis Zografou, Athens 157 71, Greece
17. COST Action: CA18212 - Molecular Dynamics in the GAS phase, Management Committee (7/10/2020-11/5/2024).
18. COST Action: CA17113 - Trapped Ions: Progress in classical and quantum applications, Management Committee (27/10/2020-17/09/2022).
19. PNNL and TPCI/NHRF project (Coordinator), contract: 628204 (5/2022-8/2022)  
Support for Scalable and Predictive methods for Excitations and Correlated phenomena: “Many-body analysis of elementary particles in the atomic nucleus.” Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens
20. Research visitor to Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, CZ, 23-25/10/2022.  
“Calculations of multiple metal centers in systems of catalytic and biological importance”, D. Tzeli
21. PROM programme, Research Visitor at Gdańsk University of Technology, Gdańsk, Poland, 27/3-1/4/2023.  
“Computational Molecular Physics and Physical Chemistry: From diatomics to supermolecular systems”, D. Tzeli (invited talk)
22. COST Action: CA22131 - Supramolecular LUMinescent Chemosensors for Environmental Security (LUCES) (16/10/2023-15/10/2027).

- **Participation as an Evaluator, Expert, and Reviewer**

1. **Reviewer and Monitor** for the European Commission (2016-2022)  
Evaluation of the proposals submitted in response to the H2020-FETOPEN-1-2016-2017, H2020-FETOPEN-2018-2019-2020-01 (work programme H2020 Future and Emerging, 2016-2020); HORIZON-EIC-2022-PATHFINDEROPEN-01; HORIZON-WIDERA-2023-ACCESS-02- Twinning  
Monitoring (review) of grant agreement: H2020-FETOPEN-2018-2019-2020-01 (2018-2024)
2. **Evaluator and Reviewer (Rapporteur)** for Romanian National Research Council (2012-2021).  
Evaluation of project proposals for Executive Agency for Higher Education, Research, Development and Innovation Funding  
PN-IV-RU-SC-TE-2023-1; PN-IV-ID-PCE-2023-1; PN-III-DCD-RU-PD-2021-3; PN-III-P4-ID-PCE-2020;

PN-II-P4-ID-PCE-2020-2; PN-III-P2-2.1-PED-2019; PN-III-P2-2.1-PED-2019; PN-III-P2-2.1-PED-2016; PN-II-RU-TE-2014; PN-II-PT-PCCA-2013; PN-II-RU-PD-2012; PN-II-ID-PCE-2012.

3. **Evaluator** of grant award procedures in natural science for the Central Coordination Unit, Council of Ministers of the Republic of Bulgaria (2017-2020)
4. **Evaluator** for Cyprus Research Promotion Foundation (RPF), RESTART 2016-2020 Programmes for Research, Technological Development and Innovation.
5. **Evaluator** of grant applications in the open call “Excellent Research” for Ministry of Education, Youth and Sports of the Czech Republic. (2022-2023)
6. **Reviewer** for the State Scholarships Foundation/ IKY, National Agency of the Erasmus+ programme in Greece for the fields of education and training (2014-2020)
7. **Reviewer** and **Evaluator** for General Secretariat for Research and Innovation (2020-)
8. **Registered Instructor** for Centre for Continuing Education and Lifelong Learning (CCE/KEDIVIM) Κέντρο Επιμόρφωσης και Δια Βίου Μάθησης (ΕΑΠ) (2022)
9. **Reviewer for the Journals:** Materials Science and Engineering: B, Applied Surface Science, International Journal of Molecular Science, Journal of Physical Chemistry A and B, European Journal of Physics, Spectroscopy Letters, Physical Chemistry Chemical Physics, Molecules, RSC Advances, Journal of Computational Chemistry, CrystEngComm, Nanoscale, Journal of Organic Chemistry, Journal of Molecular Structure, Current Microwave Chemistry, Science Journal of Chemistry, Journal of Molecular Pharmaceutics & Organic Process Research, Current Organic Chemistry, Molecular Systems Design & Engineering, Archives in Chemical Research, Medicinal Chemistry, Crystal Growth & Design, Journal of Organometallic Chemistry, Journal of Nanosciences: Current Research, Modern Chemistry & Applications, Journal of Advanced Chemical Engineering, Inorganic Chemistry, Open Chemistry, Optical materials, ChemPhysChem, Journal of Quantitative Spectroscopy and Radiative Transfer, Asian Journal of Applied Chemistry Research, Journal of Pharmaceutical Research International, Biomolecules, Asian Journal of Chemical Sciences, Physics Letters A, Catalysts, Chemosensors, ACS Omega, Symmetry, Chemical Physics, The Journal of Chemical Physics, Structural Chemistry, Life, Crystals, Journal of Composites Science, Trends in Computer Science and Information Technology, International Journal of Quantum Chemistry, PNAS, Photochemical & Photobiological Sciences, Computational and Theoretical Chemistry, Pharmaceutics, Applied Sciences, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, Inorganic Chemistry Communications.
10. **Member of the Editorial Boards** of the journals:
  - a) E-Journal of Chemistry (impact factor 2016: 1.300, 2/2012-2/2017)
  - b) International Journal of Computational and Theoretical Chemistry (2017-2020).
  - c) The Open Physics Journal (2017-2019)
  - d) The Open Access Journal of Science and Technology (2014- )
  - e) Journal of Chemical Technology and Applications (2017- )
  - f) Molecules (impact factor: 4.927) (2020- )
    - Editor of a Special Issue: Advances in Modeling of Chemical Reactions by QM/MM Calculations
    - Editor of a Special Issue: Fundamental Aspects of Chemical Bonding
  - g) Frontiers in Chemistry - Supramolecular Chemistry (Associate Editor, 2022-2024) (impact factor: 5.545)
  - h) The Journal of the Association of Greek Chemists (Section Editor 2023-)
11. **Examiner to evaluate Ph.D. Theses in India**
  - a) Faculty of Electrical Engineering, Anna University, Chennai, India
  - b) Department of Chemistry Bharathiar University, Coimbatore, Tamil Nadu, India.

- **Scientific interests**

**Computational Chemistry and Physics / Theoretical Chemistry**

- Application of a series of methodologies for accurate calculation of absorption and fluorescence spectra
- Calculation of ground & excited states, potential energy curves & surfaces, relativistic effects, transition states, reaction paths
- Analysis of chemical bonding
- Methodologies: CAS, MRCI, RCCSD(T), MP $n$  DFT, semiempirical, MD.
- Accurate ab initio calculations on molecules including transition metals.
- Study of van der Waals systems, interactions of water with “hydrophobic” organic molecules.
- Supramolecular systems, fullerene crown ethers, complexes of porphyrins, and encapsulated complexes.
- Organic reactions, reaction paths, catalysis.
- Solid state, interactions and adsorption of small molecules on surfaces.
- Magnetic nanostructures consisting of a central core and surrounded by one or various shells.
- Molecular logic gates, photoinduced charge transfer processes.
- Molecular systems/Candidates for drugs. Photosensitizer candidates for photodynamic therapy.

- **Publications**

<http://jupiter.chem.uoa.gr/pchem/pubs/tzeli.html>

[1248 citations, h-index=19, i10-index=35 (google scholar) 12/2023]

1. On the electronic structure of ground ( $X^3\Sigma^-$ ) and some low-lying excited states ( $A^3\Pi$ ,  $a^1\Delta$ ,  $b^1\Sigma^+$  and  $B^3\Sigma^-$ ) of the isovalent species P-Li and P-Na.  
D. Tzeli, A. Papakondylis and A. Mavridis, *J. Mol. Struct. (THEOCHEM)*, **417**, 277-287 (1997).
2. On the electronic structure of  $NLi_2$  and  $PLi_2$  Ground and Low-Lying excited states.  
D. Tzeli, A. Papakondylis and A. Mavridis, *J. Phys. Chem. A* **102**, 2223-2230 (1998).
3. The electronic structure of  $ScAl^+$ . Ground and Low-Lying excited states.  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **104**, 6861-6870 (2000).
4. A first principles study of the acetylene-water interaction.  
D. Tzeli, A. Mavridis and S. Xantheas, *J. Chem. Phys.* **112**, 6178-6189 (2000).
5. First principles investigation of Boron and Aluminum Carbides, BC, AlC and their Anions,  $BC^-$  and  $AlC^-$ . I  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **105**, 1175-1184 (2001).
6. Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. II.  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **105**, 7672-7685 (2001).
7. A molecular level study of the aqueous microsolvation of acetylene.  
D. Tzeli, A. Mavridis and S. Xantheas, *Chem. Phys. Lett.* **340**, 538-546 (2001).
8. Theoretical investigation of iron carbide, FeC.  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **116**, 4901-4921 (2002).
9. First Principles Examination of the Acetylene–Water clusters,  $HCCH-(H_2O)_x$   $x = 2, 3$ , and 4.  
D. Tzeli, A. Mavridis and S. Xantheas, *J. Phys. Chem. A* **106**, 11327-11337 (2002).
10. On the dipole moment of the ground state  $X^3\Delta$  of iron carbide, FeC.  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **118**, 4984-4986 (2003).
11. On the ground state of titanium phosphide, TiP: A theoretical investigation.  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **121**, 2646-2648 (2004).
12. The dipole moments of the excited states of FeC.  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **122**, 056101-2 (2005).
13. The  $CH(X^2\Pi, a^4\Sigma^-)\dots OH_2$  and  $CH_2(\tilde{X}^3B_1, \tilde{a}^1A_1)\dots OH_2$  interactions. A first principles investigation.  
D. Tzeli and A. Mavridis, *Int. J. Quantum Chemistry* **104**, 497-511 (2005).

14. First principles investigation of the electronic structure of the iron carbide cation,  $\text{FeC}^+$ .  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **109**, 9249-9258 (2005).
15. Ab initio investigation of the electronic and geometric structure of Magnesium Diboride,  $\text{MgB}_2$ .  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **109**, 10663-10674 (2005).
16. Electronic structure of cobalt carbide,  $\text{CoC}$ .  
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **110**, 8952-8962 (2006).
17. Theoretical investigation of the ground and low-lying excited states of Nickel Carbide,  $\text{NiC}$ .  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **126**, 194304(1-12), (2007).
18. Theoretical investigation on the electronic and geometric structure of  $\text{GaN}_2^+$  and  $\text{GaN}_4^+$ .  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *J. Phys. Chem. A* **111**, 8892-8902 (2007).
19. Theoretical study of adsorption of gallium and gallium nitrides on  $\text{Si}(111)$ .  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Chem. Phys. Lett.* **448**, 88-92 (2007).
20. Electronic structure and bonding of the 3d-transition metal borides,  $\text{MB}$ ,  $\text{M} = \text{Sc, Ti, V, Cr, Mn, Fe, Co, Ni}$ , and  $\text{Cu}$  through all electron *ab initio* calculations.  
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **128**, 034309(1-14) (2008).
21. The electron affinity of the gallium nitride ( $\text{GaN}$ ) and digallium nitride ( $\text{GaNGa}$ ). The importance of the basis set superposition error in strongly bound systems.  
D. Tzeli and A. A. Tsekouras, *J. Chem. Phys.* **128**, 144103(1-7) (2008).
22. Structure and Energetics of  $\text{InN}$  and  $\text{GaN}$  Dimers.  
Lucia Šimová, Demeter Tzeli, Miroslav Urban, Ivan Černušák, G. Theodorakopoulos, and I. Petsalakis  
*Chem. Phys.* **349**, 98-108 (2008) Lischka's Special Issue.
23. Theoretical study on the electronic states of  $\text{NaLi}$ .  
I. D. Petsalakis, D. Tzeli, and G. Theodorakopoulos *J. Chem. Phys.* **129**, 054306(1-11) (2008).
24. A DFT study of adsorption of gallium and gallium nitrides on  $\text{Si}(111)$ .  
D. Tzeli, G. Theodorakopoulos, and I. D. Petsalakis (Frontiers in Quantum Systems in Chemistry and Physics – PTCP, **18**, 341-350 (2008), *Proceedings of the QCSP-XII*, Ed. S. Wilson et al. Springer Science.
25. Theoretical study of the Gallium Nitride molecules,  $\text{GaN}_2$  and  $\text{GaN}_4$ .  
D. Tzeli, G. Theodorakopoulos and I. D. Petsalakis *J. Phys. Chem. A*, **112**, 8858-67 (2008).
26. First principles study of the electronic structure and bonding of  $\text{Mn}_2$ .  
D. Tzeli, U. Miranda, I. G. Kaplan, and A. Mavridis *J. Chem. Phys.* **129**, 154310 (2008).
27. Theoretical study of adsorption of group IIIA nitrides on  $\text{Si}(111)$   
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos *J. Phys. Chem. C* **113**, 5563-5567 (2009).
28. Theoretical study of adsorption of group IIIA metals on  $\text{Si}(111)$ .  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos *J. Phys. Chem. C*, **113**, 13924–13932 (2009).
29. Theoretical investigation of the ground and low-lying excited states of Gallium and Indium Silicides,  $\text{GaSi}$  and  $\text{InSi}$ .  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *J. Chem. Phys.* **131**, 234301(1-9) (2009).
30. Accurate ab initio calculations of the ground states of  $\text{FeC}$ ,  $\text{FeC}^+$ , and  $\text{FeC}^-$   
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **132**, 194312 (2010).
31. Mind the Basis Set Superposition Error  
D. Tzeli and A. A. Tsekouras, *Chem. Phys. Lett.* **496**, 42 (2010).
32. Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with  $(\text{CH}_3)_x\text{NH}_{4-x}^+$ ,  $x = 0 - 4$   
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Phys. Chem. Chem. Phys.* **13**, 954 (2011).
33. Theoretical study of different modes of binding in supramolecular complexes of exTTF with  $\text{C}_{60}$  and  $\text{C}_{59}\text{N}$   
I. D. Petsalakis, D. Tzeli, I. S. K. Kerkines, and G. Theodorakopoulos, *Comput. Theoret. Chem.* **965**, 168–175 (2011).
34. Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a  $\pi$ -extended TTF derivative  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Phys. Chem. Chem. Phys.* **13**, 11965 (2011).
35. A theoretical study of complexes of crown ethers with substituted ammonium cations  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Advances in the Theory of Quantum Systems in*

*Chemistry and Physics, - Progr. Theor. Chem. Phys.* **22** 599-610 (2011), Book of proceedings of the QSCP XV, Ed. P.E. Hoggan et al.

36. Computational Insight into the Electronic Structure and Absorption Spectra of Lithium Complexes of N-confused Tetraphenylporphyrin  
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *J. Phys. Chem. A* **115**, 11749 (2011).
37. Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes  
D. Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr *J. Am. Chem. Soc.* **133**, 16977 (2011).
38. Conformations and fluorescence of encapsulated stilbene  
D. Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr *J. Am. Chem. Soc.* **134**, 4346 (2012).
39. Encapsulated hydrogen-bonded dimers of amide and carboxylic acid  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, D. Ajami, W. Jiang and J. Rebek, Jr *Chem. Phys. Lett.* **548**, 55 (2012).
40. Theoretical study of free and encapsulated carboxylic acid and amide dimers  
D. Tzeli, G. Theodorakopoulos, I. D. Petsalakis, D. Ajami and J. Rebek, Jr *Int. J. Quantum Chem.* **113**, 734 (2013).
41. Compression in encapsulated carboxylic acid homodimers  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos Jr *Chem. Phys. Lett.* **573**, 48 (2013).
42. Theoretical study on the electronic structure, formation and absorption spectra of lithium, sodium and potassium complexes of N-confused tetraphenylporphyrin  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, *Comput. Theoret. Chem.* **1020**, 38 (2013).
43. Structural, Vibrational, Thermodynamic and Frontier Molecular Orbital Studies on (GaN)<sub>2</sub>: A DFT and MP2 Approach  
T. Mathavan, G. V. Kumari, D. Tzeli, M. A. Jothirajan, A. M. F. Baniel, S. Umapathy, *Intern. J. Scient. Eng. Research*, **5**, 29 (2014).
44. A study on thermochemical properties of ZnS Nanomaterial: A computational Approach  
T. Mathavan, A. Varghese, G. Vanitha Kumari, M. A. Jothirajan, A. M. F. Beniel, D. Tzeli, S. Umapathy, *Intern. J. Scient. Eng. Research*, **5**, 33 (2014).
45. Magnetism in the Interface of Co/CoO  
D. Tzeli, A. Morphis, J. A. Blackman, and K. N. Trohidou, *Eur. Phys. J. Web of Conferences*, **75**, 03001 (2014)
46.  $\beta$ -Nitroso-o-Quinone Methides: Potent Intermediates in Organic Chemistry and Biology. The impact of the NO group on their Structure and Reactivity Profile. A Theoretical Insight  
P. Kozielwicz, P. G. Tsoungas, D. Tzeli, I. D. Petsalakis, M. Zloh, *Struct. Chem.* **25**, 1711 (2014)
47. The role of the host-guest interactions in the relative stability of compressed encapsulated homodimers and heterodimers of amides and carboxylic acids  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, D. Ajami, J. Rebek, Jr, *Theor. Chem. Acc.* **133**, 1503 (2014)
48. Arene-Fused 1,2-Oxazole N-Oxides and Derivatives. The Impact of the N-O Dipole and Substitution on their Aromatic Character and Reactivity Profile. Can it be a Useful Structure in Synthesis? A Theoretical Insight.  
P. Kozielwicz, D. Tzeli, P. G. Tsoungas, M. Zloh, *Struct. Chem.* **25**, 1837 (2014)
49. Intramolecular Cyclization of  $\beta$ -Nitroso-o-Quinone Methides. A Theoretical Endoscopy of a Potentially Useful Innate "Reclusive" Reaction  
D. Tzeli, P. G. Tsoungas, I. D. Petsalakis, P. Kozielwicz, M. Zloh, *Tetrahedron* **71**, 359 (2015).
50. Reversible encapsulation in a covalent capsule  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, J. Rebek, Jr, *Chem. Phys. Lett.* **633**, 99 (2015)
51. Encapsulation of monomers, homodimers and heterodimers of amides and carboxylic acids in three non-covalent assemblies  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, J. Rebek, Jr, *Struct. Chem.* **26**, 1585 (2015).

52. Experimental and theoretical spectroscopic studies of branchlet-like SrCO<sub>3</sub> superarchitecture  
A. Divya, T. Mathavan, P. Arunarajeswari, J. Archana, Y. Hayakawa, D. Tzeli, A. Milton Franklin Benial, *AIP Conference Proceedings* **1731**, 050145 (2016)
53. 2, 2'-Dihydroxybenzophenones and Derivatives. Efficient Synthesis and Structure Endoscopy by DFT and NMR. Credentials as Potent Antiinflammatory Agents  
D. Tzeli, P. Kozielwicz, M. Zervou, C. Potamitis, K. Kokkotou, B. Rak, A. Petrou, E. Tsolaki, A. Gavalas, A. Geronikaki, I. D. Petsalakis, P. G. Tsoungas, *Chem Select* **1**, 2426 (2016)
54. Molecular Logic Gates based on benzo-18-crown-6 ether of styrylquinoline. A theoretical study  
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- **Other Publications**
99. Women's contributions to chemistry (Η συνεισφορά των γυναικών στη Χημεία)  
D. Tzeli, *Chimica Chronika* **73**(5), 22 (2011).
100. Application of Quantum Mechanics/Molecular Mechanics Methodologies to Metalloproteins  
C. E. Tzeliou, M. A. Mermigki, D. Tzeli, *Encyclopedia* (2022) <https://encyclopedia.pub/entry/22516>
101. Molecular logic gates  
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102. Electronic Structure and Chemical Bonding of Transition-Metal Monoborides  
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- **Books**

103. Translation & Editing in Greek of Chapter 13: *Molecular Electronic Structure and the Chemical Bond*, Physical Chemistry for the Chemical Sciences *written by* Raymond Chang and John W. Thoman Jr. Publisher: University Science Books, Royal Society of Chemistry, 2014  
Greek Publisher: Broken Hill Publishers LTD, Cyprus
104. Translation & Editing in Greek of Chapter 12: *Atoms and Molecules*, Physical Chemistry *written by* David W. Ball with contributions by Tomas Baer  
Publisher: Cengage Learning, 2<sup>nd</sup> Edition, USA, 2015  
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- **Presentation and Participation at Conferences / Invited Talks**

1. *NATO ASI, "Recent Theoretical and Experimental Advances in Hydrogen-Bonded Clusters"*  
Elounda, Crete, Greece, 22/6-4/7/1997.
2. *NATO ASI, "Quantum Monte Carlo in Physics and Chemistry"*  
Summer School, Cornell University, Ithaca, N.Y., 13-24/7/1998.
3. *NATO ASI, "Metal-Ligand Interactions in Chemistry Physics and Biology"*  
Cetrano (CS), Calabria, Italy, 1-12/9/1998.  
Poster: "The electronic structure of  $\text{ScAl}^+$  Ground and Low-Lying states" D. Tzeli, A. Mavridis
4. *Fourth European Workshop on Quantum Systems in Chemistry and Physics*,  
Marly-le-Roi, Paris, France, 22-27/4/1999.  
Poster: "An ab initio investigation of the acetylene-water  $\text{HCCH}(\text{H}_2\text{O})_x$ ,  $x = 1, 2, 3, 4$  system" D. Tzeli, A. Mavridis, S. Xantheas
5. *23<sup>rd</sup> International Workshop on Condensed Matter Theories*,  
Ithaca, Greece, 17-23/6/1999.  
Invited Talk: "Quantitative Calculations on Small Molecules by ab initio methods". A. Mavridis and D. Tzeli  
Poster: "The van der Waals interaction of the acetylene molecule with water clusters,  $\text{C}_2\text{H}_2(\text{H}_2\text{O})_x$   $x = 1, 2, 3$  and 4" D. Tzeli, S. Xantheas and A. Mavridis.
6. *Fifth European Workshop on Quantum Systems in Chemistry and Physics*,  
Uppsala University, Sweden, 13-18/4/2000.  
Poster: "On the Electronic Structure of Iron Carbide,  $\text{FeC}$ . Ground and 35 Low-Lying Excited States" D. Tzeli and A. Mavridis
7. *Sixth European Workshop on Quantum Systems in Chemistry and Physics*,  
Sofia, Bulgaria, 19-24/4/2001.  
Poster: "On the Electronic Structure of Iron Carbide,  $\text{FeC}$ . Ground and 35 Low-Lying Excited States" D. Tzeli and A. Mavridis
8. *Eighth European Workshop on Quantum Systems in Chemistry and Physics*,  
Spetses, Greece, 30/8 – 4/9/2003. (Organizing Committee)  
Poster: "First Principles Investigation of the magnesium diboride  $\text{MgB}_2$ " D. Tzeli and A. Mavridis  
Poster: "On the Electronic Structure of Iron Carbide Cation,  $\text{FeC}^+$ . Ground and 39 Low-Lying Excited States" D. Tzeli and A. Mavridis
9. *Molecular Quantum Mechanics: The No Nonsense Path to Progress*  
International Conference in honour of Nicholas C. Handy  
St. John's College, Cambridge University, England, 24 – 29/7/2004.  
Poster: "On the Electronic Structure of Cobalt Carbide,  $\text{CoC}$ . Ground and Low-Lying Excited States" D. Tzeli and A. Mavridis
10. *Lecture at the Theoretical Chemistry Department, Materials Science Center, Rijksuniversiteit Groningen, the Netherlands 28/10/2004.*  
"Theoretical study of the Magnesium Diboride molecule,  $\text{MgB}_2$ ", D. Tzeli
11. *Lecture at the National Hellenic Research Foundation, Athens, Greece, 7/12/2006.*  
"Spectroscopic parameters and electronic structure of metal-borides and metal-carbides via ab initio calculations", D. Tzeli

12. *Lecture* at the Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University, Mlynská dolina, Bratislava, Slovakia, 27/6/2007.  
 “Ab initio investigation of small and large systems. a. Gallium nitrides and their adsorption on Si(111). b. First row transition Metal Borides, MB, M = Sc - Cu.”, D. Tzeli
13. *Quantum Systems in Chemistry and Physics, Workshop, QSCP XII*  
 Royal Holloway, University of London, U.K., 30/8 – 5/9/2007.  
 Poster: Theoretical study of adsorption of gallium and gallium nitrides on Si(111). D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos  
 Talk: “Theoretical investigation of the First row transition Metal Borides, MB, M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni and Cu”. D. Tzeli and A. Mavridis
14. *Cnano '09 International Conference on Carbon Nanostructured Materials*  
 Santorini, Greece, 4 – 8/10/2009 (*Organizing Committee*)  
 Poster: “Theoretical study of different modes of binding in supramolecular complexes of ex-TTF with C<sub>60</sub> and C<sub>59</sub>N” I. D. Petsalakis, D. Tzeli, N. Tagmatarchis, G. Rotas and G. Theodorakopoulos  
 Poster: “Theoretical study of the spectrum of Fullerene crown ethers” D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos
15. *Lecture* at the Department of Theoretical Chemistry, Bergische University GH Wuppertal, Germany, 9/6/2010.  
 “Electronic structure and surface adsorption of molecules containing group IIIA elements”, D. Tzeli
16. *International Workshop of Quantum Systems in Chemistry and Physics (QSCP-XV)*  
 Cambridge, UK, 31/8 – 5/9/2010.  
 Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with (CH<sub>3</sub>)<sub>x</sub>NH<sup>+</sup><sub>4-x</sub>, x = 0 – 4” D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos
17. *Fullerene Silver Anniversary Symposium – FSAS 2010, (Organizing Committee)*  
 Crete, Hellas, 4 – 10/10/2010.  
 “Theoretical study of the spectrum of complexes of Fullerene crown ethers with  $\pi$ -Extended TTF Derivatives” D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos
18. *14<sup>th</sup> International Density Functional Theory Conference: Applications in Physics, Chemistry, Biology, Pharmacy, (Organizing Committee)*  
 Demokritos, Athens, Greece, 29/8 – 2/9/2011.  
 “Encapsulation complexes of amide, boronic acid and carboxylic acid dimers: Theoretical study of hydrogen bonding.” D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, and J. Rebek, Jr.
19. *International conference on Advanced Materials, Processing and Devices (AMPD – 2013)*  
 Department of Materials Science, Madurai Kamaraj University, India  
 “Investigations on Homo-Lumo energy and thermochemical properties of (GaN)<sub>2</sub>” G. Vanitha, T. Mathavan, D. Tzeli, M. A. Jothirajan, S. Umapathy, A. M. F. Baniel
20. *JEMS (Joint European Magnetic Symposia) 2013*  
 Rhodes, Greece, 25-30/8/2013  
 “Magnetism in the interface of Co/CoO” D. Tzeli, A. Morphis, J. A. Blackman, K. N. Trohidou
21. *29<sup>th</sup> XXIX Panhellenic Conference on Solid-State Physics and Materials Science*  
 National Technical University of Athens, Greece, 22-25/9/2013  
 “Magnetism in binary and encapsulated Co-O clusters”, D. Tzeli, A. Morphis, J. A. Blackman, K. N. Trohidou
22. *International Conference on "Recent Advances in Physics for Interdisciplinary Developments (ICRAPID-14)"*  
 Sathyabama University, India, 23 -24/1/2014.  
 “A study on thermochemical properties of ZnS Nanomaterial: A computational Approach”, T. Mathavan, A. Varghese, G. Vanitha Kumari, M. A. Jothirajan, A. M. F. Beniel, D. Tzeli, S. Umapathy
23. *European Materials Research Society (E-MRS) Fall Meeting 2014,*  
 Warsaw University of Technology, Poland, 15-19/9/2014  
 “Atomic scale modelling of magnetic nanoparticles: Surface and Interface effects”  
 Computer modelling in nanoscience and nanotechnology: an atomic-scale perspective III”, K.N. Trohidou, M. Vasilakaki, G. Margaris, D. Tzeli

24. *PRACE Autumn School in HPC Programming Techniques*  
Center of the Hellenic Telecommunications Organization (OTE Academy), Athens, Greece, 25-28/11/2014
25. *Invited Talk, Department of Chemistry*, National and Kapodistrian University of Athens, Greece, 30/4/2015  
“Computational Chemistry: From Diatomics to Nanoclusters”, D. Tzeli
26. Lecture at the National Hellenic Research Foundation, Athens, Greece, 2/7/2015  
“Theoretical studies on supramolecular systems”, D. Tzeli
27. *DAE SOLID STATE PHYSICS SYMPOSIUM 2015*  
Uttar Pradesh, India, 21-25/12/2015  
“Experimental and theoretical spectroscopic studies of branchlet-like SrCO<sub>3</sub> superarchitecture” A. Divya, T. Mathavan, P. Arunarajeswari, J. Archana, Y. Hayakawa, D. Tzeli, A. Milton Franklin Benia
28. *COST EUSPEC MP1306: Modern Tools for Spectroscopy on Advanced Materials*  
Athens, Greece, 13-14/2/2017  
“Predicting spectroscopic parameters in molecular logic gates” D. Tzeli
29. *Lecture at the Physics Department of the Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa*, Lisbon, Portugal, 20/4/2017.  
“Computational-Theoretical Chemistry: From diatomic molecules to nanomaterials. Prediction of their spectroscopic parameters, D. Tzeli
30. *1<sup>st</sup> International Symposium on Quantum Science and Technology*  
Aberdeen, UK, 24-27/2018  
D. Tzeli: Member of Scientific Committee of the Conference  
“Photoinduced charge-transfer in tertiary amine-fluorophore systems” (poster) D. Tzeli, Th. Mercouris, G. Theodorakopoulos, I. D. Petsalakis
31. *Theoretical Physical Chemistry / Theoretical Material Science Symposium*  
*Lecture at TPCI/NHRF*, Athens, Greece, 28/6/2018  
“Computational-Theoretical Chemistry: From diatomic molecules to supermolecular systems and materials” D. Tzeli
32. *Energy Landscapes 2018*  
Kalamata, Greece, 2-9/9/2018  
“Making molecular logic gates and sensors by inducing photophysical processes” (talk) D. Tzeli
33. *VI-SEEM NAT-GR LS+: 2018 NWChem Workshop*  
Athens, Greece, 10-11/9/2018  
Organizing Committee
34. *11<sup>th</sup> Swedish-Hellenic Life Science Research Conference*  
*NHRF*, Athens, Greece, 4-5/10/2018
35. *Athens Conference on Advances in Chemistry (acac2018)*  
National and Kapodistrian University of Athens, Athens, Greece, 30/10-2/11/2018  
“Molecular logic gates and sensors” (talk) D. Tzeli
36. *Artificial Photosynthesis Faraday Discussion*  
Cambridge, United Kingdom, 25-27/3/2019  
“Theoretical studies on the photocatalytic hydrogen production mechanism by molecular copper complexes” M. Drosou, G. Ioannidis, D. Tzeli, C. A. Mitsopoulou” (poster)
37. *Lecture at the Department of Physics, NKUA*, 27/3/2019  
“Computational Molecular Physics and Physical Chemistry”, D. Tzeli
38. *12<sup>th</sup> Swedish-Hellenic Life Science Research Conference*  
*NHRF*, Athens, Greece, 10-11/10/2019
39. *MOLPRO2016 Online Seminars*  
University of Washington, USA, 4-19/3/2020. D. Tzeli (Instructor)  
National and Kapodistrian University of Athens, GR, 2-23/12/2020. D. Tzeli (Instructor)
40. *New horizons in density functional theory Faraday Discussion*  
Faraday Division of the Royal Society of Chemistry, Online conference, 2-4 September 2020.

- “DFT study of the photophysical processes of bodipy derivatives eliciting molecular logic gate response  
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos
41. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
“Encapsulation in Chalcogen-Bonded vs Hydrogen-Bonded Cages  
D. Tzeli (Talk)
  42. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
"Analysis of the double, quadruple and sextuple chemical bonding of diatomic molecules of 2<sup>nd</sup> row transition metals"  
A. Androutsopoulos, T. Depastas, I. Karapetsas, D. Tzeli (Flash oral presentation)
  43. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
“Tuning the absorption spectra of Nickel and Zinc Complexes of N-confused Tetraphenylporphyrin”  
E. Papamichalis, I. D. Petsalakis, D. Tzeli (Flash oral presentation)
  44. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
“Theoretical study of the photophysical processes of a three-input AND molecular logic gate with an enhanced fluorescent output”  
C. Tzeliou, D. Tzeli (Flash oral presentation)
  45. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
“Electronic structure and Bonding properties of iron–sulfur clusters”  
M. A. Mermigki and D. Tzeli (Flash oral presentation)
  46. *Athens Conference on Advances in Chemistry (acac2020)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 10-14/3/2021  
“Unrevealing the catalytic mechanism of proton reduction by a copper(I) diamine catalyst”  
M. Drosou, F. Kamatsos, G. Ioannidis, A. Zarkadoulas, C. A. Mitsopoulou, C. Papatriantafyllopoulou, D. Tzeli (Talk)
  47. *MD-GAS WG1 & WG2 Meeting*  
COST Action: CA18212 - Molecular Dynamics in the GAS phase. Virtual Conference, 15-19 March 2021.  
“Time-evolution study of photoinduced charge-transfer in fluorophore systems”  
D. Tzeli, Th. Mercouris, G. Theodorakopoulos, I. D. Petsalakis (Poster presentation)
  48. *Multiscale modelling of materials and molecules - physics-based and data-driven.*  
eSSENCE-EMMC e-Meeting 7-8/6/2021.  
"Theoretical study of the photophysical processes of three-input AND molecular logic gates",  
C. Tzeliou, D. Tzeli, G. Theodorakopoulos, and I. D. Petsalakis (Poster)
  49. VI-EGAS52, 52<sup>nd</sup> Conference of the European Group of Atomic Systems, Virtual Conference, Zagreb, Croatia (6-8/7/2021)  
“Electronic structure and Bonding Properties of Diatomic Molecule FeS”  
M. A. Mermigki and D. Tzeli (Poster)
  50. VI-EGAS52, 52<sup>nd</sup> Conference of the European Group of Atomic Systems, Virtual Conference, Zagreb, Croatia (6-8/7/2021)  
“Accurate theoretical study of the spectroscopic properties of diatomic molecules including 2<sup>nd</sup> row transition metals”  
A. Androutsopoulos, T. Depastas, I. Karapetsas, D. Tzeli (Poster)
  51. *MD-GAS Cost Action 2<sup>nd</sup> General Meeting*  
COST Action: CA18212 - Molecular Dynamics in the GAS phase. Virtual Conference, 4-8 October 2021  
“The effect of acidity, oxidisability, metal coordination, light, and solvent polarity”  
C. Tzeliou, D. Tzeli
  52. *MD-GAS Cost Action 2<sup>nd</sup> General Meeting*  
COST Action: CA18212 - Molecular Dynamics in the GAS phase. Virtual Conference, 4-8 October 2021

- “Modulation of the absorption spectra of Metal Complexes of N-confused Tetraphenylporphyrin”  
E. Papamichalis, I. D. Petsalakis, D. Tzeli
53. 1<sup>st</sup> SYMPOSIUM OF GRADUATE STUDENTS OF THE CHEMISTRY DEPARTMENT  
National and Kapodistrian University of Athens, Athens, Greece, 17-18/3/2022  
“Conformational properties of new thiosemicarbazone and thiocarbohydrazone derivatives and their possible targets”  
N. Georgiou, A. Katsogiannou, D. Tzeli, S. Vassiliou, T. Mavromoustakos
54. 1<sup>st</sup> SYMPOSIUM OF GRADUATE STUDENTS OF THE CHEMISTRY DEPARTMENT  
National and Kapodistrian University of Athens, Athens, Greece, 17-18/3/2022  
“Computational Study of Fe<sub>x</sub>S<sub>y</sub> clusters”  
M. A. Mermigki, D. Tzeli
55. 1<sup>st</sup> SYMPOSIUM OF GRADUATE STUDENTS OF THE CHEMISTRY DEPARTMENT  
National and Kapodistrian University of Athens, Athens, Greece, 17-18/3/2022  
“Theoretical investigation of MoO”  
A. Androutsopoulos, T. Depastas, D. Tzeli
56. 1<sup>st</sup> SYMPOSIUM OF GRADUATE STUDENTS OF THE CHEMISTRY DEPARTMENT  
National and Kapodistrian University of Athens, Athens, Greece, 17-18/3/2022  
“The Bonding and Spectroscopy of MoC, Mo<sub>2</sub> and Mo<sub>2</sub>Cl<sub>n</sub> (n=2-10): An ab initio study”  
T. Depastas, A. Androutsopoulos, D. Tzeli
57. 1<sup>st</sup> SYMPOSIUM OF GRADUATE STUDENTS OF THE CHEMISTRY DEPARTMENT  
National and Kapodistrian University of Athens, Athens, Greece, 17-18/3/2022  
“A 3-input AND molecular logic gate with enhanced fluorescence output: The key atom for the accurate prediction of the spectra”  
C. Tzeliou, D. Tzeli
58. Lecture at the Department of Chemistry, NKUA, 20/5/2022  
“Progress in electronic-structure based computational methods: From small molecules to supermolecular systems”, D. Tzeli
59. Lecture at the Department of Chemistry, University of Patras, 26/5/2022  
“Progress in electronic-structure based computational methods: From small molecules to supermolecular systems”, D. Tzeli
60. 2<sup>nd</sup> BRFAA Mini Symposium: *Computational methods in drug and materials design*  
Biomedical Research Foundation of the Academy of Athens, Athens, 20/6/2022  
“DFT and Semiempirical Calculations: Powerful tools for drug and materials”  
D. Tzeli (Talk)
61. *Athens Conference on Advances in Chemistry (acac2022)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
(Organizing Committee)  
“Electronic structure and bonding properties of iron-sulfur model complexes: [Fe(SMe)<sub>4</sub>]<sup>q</sup>, [Fe<sub>2</sub>S<sub>2</sub>(SMe)<sub>4</sub>]<sup>q</sup>, [Fe<sub>3</sub>S<sub>4</sub>(SMe)<sub>3</sub>]<sup>q</sup>, & [Fe<sub>4</sub>S<sub>4</sub>(SMe)<sub>4</sub>]<sup>q</sup>”  
D. Tzeli (Talk)
62. *Athens Conference on Advances in Chemistry (acac2022)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
“First-principles exploration of the MoX (X = Li, Be, B, C, N, O, F) diatomic molecules”  
A. Androutsopoulos, T. Depastas, D. Tzeli (Poster)
63. *Athens Conference on Advances in Chemistry (acac2022)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
“The effect of transition metals on the absorption spectra of metallocene-naphthalimide derivatives”  
C. Tzeliou, D. Tzeli (Poster)
64. *Athens Conference on Advances in Chemistry (acac2022)*  
Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
“Computational Study of triatomic FeS<sub>2</sub> and MoS<sub>2</sub> molecules”  
M. A. Mermigki, I. Karapetsas, D. Tzeli (Poster)

65. *Athens Conference on Advances in Chemistry (acac2022)*  
 Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
 “Structure assignment, conformational analysis and discovery of potential targets of the thiosemicarbazone and thiocarbohydrazone derivatives”  
 N. Georgiou, A. Katsogiannou, D. Tzeli, S. Vassiliou, U. Javornik, J. Plavec, T. Mavromoustakos (Flash oral presentation)
66. *Athens Conference on Advances in Chemistry (acac2022)*  
 Department of Chemistry, National and Kapodistrian University of Athens, Athens, Greece, 26/6-1/7/2022  
 “Molecular studies on lipoxygenase enzyme and its potent inhibitors”  
 E. Chontzopoulou (Talk), C. Papaemmanouil, M. V. Chatziathanasiadou, D. Kolokouris, S. Kiriakidi, A. Konstantinidi, I. K. Kostakis, E. D. Chrysina, D. Hadjipavlou-Litina, D. Tzeli, A. G. Tzakos, J. Jose Nogueira Perez, T. Mavromoustakos
67. *WATOC 2020*, the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada, 3-8/7/2022.  
*The Many-Body Expansion in Chemistry*  
 S. S. Xantheas (Invited Speaker), J. Heindel, K. M. Herman, J. Mato, D. Tzeli
68. *WATOC 2020*, the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada, 3-8/7/2022.  
*The Many-Body Expansion in Alkaline Earth Metals*  
 J. Mato, D. Tzeli, S. S. Xantheas (Poster)
69. *DEEP-GAS 2022: Dynamics of Energetic & Electronic Processes in molecules and clusters in the GAS phase*  
 Madrid, Spain, 4-7/10/2022  
*Quadruple and sextuple bonds in diatomic molecules*  
 D. Tzeli (Invited Speaker), T. Depastas and A. Androutsopoulos
70. *DEEP-GAS 2022: Dynamics of Energetic & Electronic Processes in molecules and clusters in the GAS phase*  
 Madrid, Spain, 4-7/10/2022  
*The key atom for the accurate prediction of the absorption and emission spectra of a 3-input AND molecular logic gate*  
 C. E. Tzeliou, D. Tzeli (Poster)
71. Research Visitor at Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, CZ, 23-25/10/2022.  
 “Calculations of multiple metal centers in systems of catalytic and biological importance”, D. Tzeli
72. 19th Hellenic Symposium on Medicinal Chemistry, University of Patras, Patra, Greece, 9-11/3/2023  
 “Conformational properties and biological targets of thiocarbohydrazone and chalcone-derived 3,4-dihydropyrimidine thione”  
 N. Georgiou, E. Chontzopoulou, A. Cheilari, A. Katsogiannou, D. Karta, K. Vavougyiou, D. Hadjipavlou-Litina, U. Javornik, J. Plavec, D. Tzeli, S. Vassiliou, T. Mavromoustakos (Poster)
73. 7<sup>th</sup> International conference on Nanoscience and Nanotechnology ICONN-2023, SRM University, Tamil Nadu, India, 27-29/3/2023  
 “Theoretically study of the photophysical properties of the Zinc-N-Confused Tetraphenylporphyrin adsorbed or chemically linked on 2D-MoS<sub>2</sub> surface”  
 E. Papamichalis, N. N. Lathiotakis, D. Tzeli
74. 7<sup>th</sup> International conference on Nanoscience and Nanotechnology ICONN-2023, SRM University, Tamil Nadu, India, 27-29/3/2023  
 “Theoretical study of the adsorption, capture and decomposition of N<sub>2</sub>O molecule on 2D-MoS<sub>2</sub> surface with and without S-vacancies”(Kawazoe Prize for the Best Poster in ACCMS Symposium on Computational Materials, Methods and Numerical Techniques)  
 C. E. Tzeliou, N. N. Lathiotakis, D. Tzeli
75. Research Visitor at Gdańsk University of Technology, Gdańsk, Poland, 27/3-1/4/2023. (PROM programme)  
 “Computational Molecular Physics and Physical Chemistry: From diatomics to supermolecular systems”,  
 D. Tzeli (invited speaker)
76. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
 National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023



- “Computational study on the role of sulfur vacancy in 2D-MoS<sub>2</sub> surface: adsorption and reactions of the N<sub>2</sub>O molecules on a 2D-MoS<sub>2</sub> surface”  
C. E. Tzeliou, N. N. Lathiotakis, D. Tzeli
77. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Spectroscopic and Computational Studies on the Formation of Halogen-Bonded Complexes between Tertiary Amines and Halomethanes in Solution”  
E. A. Routsis, O. G. Mountanea, C. Mantzourani, C. G. Kokotos, D. Tzeli, G. Kokotos
78. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Photoorganocatalytic N-O bond cleavage of O-benzyl hydroxamic acids”  
A.-D. Gerogiannopoulou, E. A. Routsis, D. Tzeli, C. G. Kokotos, G. Kokotos
79. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Cu complexes with remote N-Heterocyclic Carbene ligands: A Theoretical and Experimental mating”  
K.P. Zois, E. Papangelis, N. Tsoureas, L. Karmazin, P. Braunstein, A. Danopoulos, D. Tzeli
80. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Synthesis and characterization of a series of 3d-metal complexes supported by a bis-aryloxide ligand”  
I. Vagiakos, D. Tzeli and N. Tsoureas
81. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Computational study of Curcumin photosensitizer for photodynamic therapy”  
E. Dimou and D. Tzeli (poster)
82. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“Computational and Experimental Study of Photochemical Processes of Dyes and Pigments Dyes-PMMA”  
C. Kolokytha, A. Sinani, T. Manouras, E. Angelakos, N. N. Lathiotakis, C. Riziotis, D. Tzeli (poster)
83. 2<sup>nd</sup> Symposium of Graduate Students of the Chemistry Department  
National and Kapodistrian University of Athens, Athens, Greece, 8-9/6/2023  
“In silico study and synthesis of statins and novel magnetic nanocarriers for targeting vascular therapies”  
K. Moschovou, D. E. Prokopiou, A. Stavropoulou, N. Georgiou, D. Tzeli, P. Neofytou, E. Efthimiadou, T. Mavromoustakos (poster)
84. 17<sup>th</sup> International congress of Quantum Chemistry, ICQC 2023, Bratislava, Slovakia, 26/6-1/7/2023  
“Electronic structure and bonding properties of iron-sulfur model complexes”  
D. Tzeli, C. Mejuto-Zaera, D. Williams-Young, N. M. Tubman, M. Matoušek, J. Brabec, P. Golub, L. Veis, S. Raugei, S. S. Xantheas, W. A. de Jong (invited oral presentation)
85. MD-GAS Training school: Theory and modelling of dynamics of molecules and clusters in the gas phase, Gdańsk, Poland, 3-7/7/2023  
“Theoretical study of adsorption and chemisorption of N<sub>2</sub>O molecules on a 2D-MoS<sub>2</sub> surface: the effect of S-vacancies”  
C. E. Tzeliou, N. N. Lathiotakis, D. Tzeli
86. MD-GAS Training school: Theory and modelling of dynamics of molecules and clusters in the gas phase, Gdańsk, Poland, 3-7/7/2023  
“UV-VIS, NMR and DFT studies on the formation of halogen-bond between tertiary amines and CBr<sub>4</sub> in solution”  
E. A. Routsis, O. G. Mountanea, D. Tzeli, C. G. Kokotos, G. Kokotos
87. EuChemS CompChem: European Chemical Society Division of Computational and Theoretical Chemistry, Thessaloniki, 27-31/8/2023  
“Electronic Structure and Chemical Bonding in systems containing of transition metals”  
D. Tzeli (invited talk)

88. SSD20 - 20th International Conference on Solid State Dosimetry, Viareggio, Italy, 17-22/9/2023.  
 "A preliminary Ab Initio study of Thermoluminescence properties in Beryllium Oxide: Theoretical investigation on the electronic states of BeO: Mg<sup>2+</sup>, Si<sup>4+</sup> and BeO: Cr<sup>3+</sup>, Mg<sup>2+</sup>"  
 E. Tsoutsoumanos, D. Tzeli, A. Avramopoulos, P.G. Konstantinidis, N. Laskaris, N. Lathiotakis, G. Kitis, G.S. Polymeris, T. Karakasidis (poster)
89. XXXVII Panhellenic Conference on Solid State Physics and Materials Science, Thessaloniki, Greece, 17-20/9/2023  
 "Investigating Thermoluminescence Signal Replication in BeO:Mg<sup>2+</sup>, Si<sup>4+</sup> via First Principles Computational Analysis"  
 E. Tsoutsoumanos, D. Tzeli, A. Avramopoulos, P.G. Konstantinidis, N. Laskaris, N. Lathiotakis, G. Kitis, G.S. Polymeris, T. Karakasidis (poster)
90. 4<sup>th</sup> MD-GAS General Meeting, Dubrovnik, Croatia, 25-27/9/2023  
 "Theoretical study of Fe<sub>x</sub>S<sub>y</sub> and MoS<sub>y</sub> molecular systems"  
 D. Tzeli and M. A. Mermigki (poster)
91. 4<sup>th</sup> MD-GAS General Meeting, Dubrovnik, Croatia, 25-27/9/2023  
 "Computational study on the thermochemistry and chemical bonding of the HN<sub>3</sub>, H<sub>2</sub>N<sub>4</sub>, HNC<sub>2</sub><sup>2-</sup> and H<sub>2</sub>N<sub>2</sub>C<sub>2</sub><sup>2-</sup> species"  
 G. A. Tsekouras and D. Tzeli (poster)
92. 4<sup>th</sup> MD-GAS General Meeting, Dubrovnik, Croatia, 25-27/9/2023  
 "Theoretical kinetic study of Criegee intermediates with N<sub>2</sub>O"  
 C. E. Tzeliou, E. Erdmann, D. Tzeli, and M. Łabuda (talk)
93. 2<sup>nd</sup> Panhellenic Workshop on Inorganic Chemistry, Chemistry Department, NKUA, Athens, GR, 28-30/9/2023  
 "Theoretical and Experimental perspectives on Cu complexes bearing remote N-Heterocyclic Carbene ligands (rNHC's)"  
 K.P. Zois, E. Papangelis, P. Braunstein, L. Karmazin, N. Tsoureas, A. Danopoulos, D. Tzeli
94. 9<sup>th</sup> International BAU Drug Design Congress 2023, Constantinoupolis, Turkey, 29/11-2/12, 2023  
 "A 4-hydroxy-2-quinolinone-triazole hybrid as potential anti-inflammatory agent"  
 N. Georgiou, A. Tzani, I. Kostopoulou, M.-A. Karadendrou, K. Vavougyiou, P. Sket, J. Plavec, D. Tzeli, A. Detsi, Th. Mavromoustakos
95. Lecture at the Department of Chemistry, University of Ioannina, Ioannina, 23/11/2023  
 "Electronic structure methodology: From small molecules to supermolecular systems", D. Tzeli

• **Presentations and Invited Talks at General Public Conferences**

1. "*Chemistry Experiments for pre-school children*".  
 National and Kapodistrian University of Athens, Kindergarten, 21/11/2006, D. Tzeli
2. Event: "*Miraculous ... Chemistry*". Organization: Centre for Women and Karditsa 1<sup>st</sup> Lyceum, under the auspices of the GSGE, the Municipality of Karditsa, Department of Secondary Education Karditsa and the Union of Greek Chemists Regional Department of Thessaly, Karditsa, 3/5/2011.  
 "Women's contributions to chemistry", D. Tzeli (invited talk)
3. *Researcher's Night*, NCSR Demokritos, 27/9/2013  
 "Monte Carlo Simulations of the magnetic behavior of magnetic nanocomposites and nanoparticles and Electronic Calculations of magnetic nanoparticles for their use in biomedicine applications (magnetic hyperthermia), in magnetic recording, and in magnetic quantum dots", M. Vasilakaki, D. Tzeli, A. Morphis, K.N. Trohidou
4. 1<sup>st</sup> *Athens Science Festival*, Technopolis Municipality of Athens, 30/4-4-5/2014  
 "Computational and Theoretical Physics and Chemistry", D. Tzeli (invited talk)
5. *Academic and professional careers in natural sciences: Opportunities, challenges and the role of Gender*, ELEGYP, Department of Informatics, NKUA, 30/10/2014"  
 "Professional career in natural sciences", D. Tzeli
6. *Woman in research: problems - causes - prospects*, NHRF, Athens, Greece, 17/3/2016.

7. *Athens Science Festival*, Technopolis, Gazi, 24-29/4/2018  
"Chemical Experiments via computer", D. Tzeli, 27/4/2018.
8. *Athens Science Festival*, Technopolis, Gazi, 24-29/4/2018  
Women in Science, Union of Greek Chemists  
"Women in Science: Working women and mothers in Science", D. Tzeli, 28/4/2018. (invited talk)
9. *Anniversary Exhibition «Το Θηλυκό Πρόσωπο της Επιστήμης» ("The female identity of Science")*,  
*Celebration for the 20 years of L'ORÉAL-UNESCO For Women in Science program*, 20-23/9/2018  
"Computational Chemistry: Molecular Switches", D. Tzeli, 22/9/2018. (invited talk)
10. *Up Event 2018: Ημέρες Καριέρας*, Technopolis, Gazi, 13-14/10/2018  
"Research in Natural Science", D. Tzeli, 14/10/2018 (invited talk)
11. *Workshop "Educational career guidance"*, *Leonteios Lycee Nea Smyrni*,  
"Profession: Chemist", D. Tzeli, 25/02/2021 (talk)
12. *IUPAC Global Women's Breakfast*, Department of Chemistry, NKUA, Athens, Greece  
"Women in Science: Empowering Diversity in Science", D. Tzeli, 16/02/2022 (talk)

- **Professional Affiliations**

1. Association of Greek Chemists    2. Hellenic Mathematical Society

- **Computer skills**

1. Operating Systems: Unix, Windows, MacOS; 2. Applications: MS Office, Origin, Igor, Corel Draw, Chem Office, MatLab, etc.; 3. FORTRAN, PERL; 4. Codes: MOLPRO, GAUSSIAN, NWChem, MOLCAS, ORCA, COLOMBUS, MELD, Gamess, TURBOMOLE, GROMACS, VASP, SIESTA, FLEUR, Quantum Espresso.

- **Languages**

1. Greek (mother tongue) 2. English (excellent, C2 level) 3. German (intermediate level) 4. French (intermediate level) 5. Japanese (elementary level) 6. Spanish (elementary level)