

# Demeter Tzeli



Associate Professor

LAB OF PHYSICAL CHEMISTRY, DEPARTMENT OF CHEMISTRY, NATIONAL AND KAPODISTRIAN UNIVERSITY OF ATHENS

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(citations:1248, h-index:19, i10-index:35)

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## EDUCATION

- 1995 Bachelor in Chemistry, Dept of Chemistry, NKUA, GR
- 1997 Master in Physical Chemistry / Dept of Chemistry, NKUA / Thesis Title: "Ab initio calculations on P-X and Y-Li<sub>2</sub> molecular systems, where X=Li, Na and Y=N, P".
- 2000 PhD in Quantum Chemistry / Dept of Chemistry, NKUA / Thesis Title: I. Structure and interaction energy of the van der Waals systems C<sub>2</sub>H<sub>2</sub>(H<sub>2</sub>O)<sub>x</sub>, x = 1 - 4 and CH<sub>y</sub>-H<sub>2</sub>O, y = 1 and II. Electronic structure of the carbides BC, BC<sup>-</sup>, HBC, AIC, AIC<sup>-</sup> and HAIC via ab initio calculations.

## RESEARCH FIELDS

### Theoretical and Computational Chemistry

- Accurate ab initio calculations on molecules including transition metals.
- Supramolecular systems: Fullerene crown ethers, complexes of porphyrins, encapsulated complexes.
- van der Waals systems.
- Organic reactions, reaction paths, catalysis.
- Solid state: Interactions and adsorption of small molecules on surfaces, magnetic nanostructures.
- Molecular logic gates, sensors, photoinduced charge transfer processes.
- Candidates for drugs. Photosensitizer candidates for photodynamic therapy.
- Theory

## EDUCATIONAL EXPERIENCE

### UNDERGRADUATE COURSES

- Physical Chemistry Laboratory II (514) / Compulsory / Department of Chemistry / (1 h/w + 4 lab h/w)
- Physical Chemistry Laboratory III (614) / Compulsory / Department of Chemistry / (4 lab h/w)
- Materials Chemistry (703) / Elective / Department of Chemistry / (4 h/w)
- Physical Chemistry (Δ405) / Compulsory / Department of Pharmacy / (3 h/w + 2 lab h/w)

### GRADUATE COURSES

- Molecular Quantum Chemistry Methodologies / Master Program in Physical Chemistry / Lab of Physical Chemistry / Department of Chemistry /
- Research Methodology & Laboratory Practice in Physical Chemistry – Bibliographic Research / Master Program in Physical Chemistry / Lab of Physical Chemistry / Department of Chemistry /

## DISCRIMINATIONS / SCHOLARSHIPS

- Fellowship of Academy of Athens (9/2002-6/2004)
- HPC- Europa Transnational Access programme (10-11/2004)
- FP7-Capacities-Research Potential Of Convergence Regions (5/2008-1/2011)
- Greek Award 2009 L'ORÉAL-UNESCO for the Women in Science.

## RESEARCH GRANTS

- AWU program / PhD fellow / Pacific Northwest National Laboratory, Richland, U.S.A / 7-9/1998.
- SSATES, EPEAEK / National Resources / 5/1999-12/1999
- Academy of Athens / PI, NKUA / Academy of Athens funding / 9/2002-6/2004
- Pythagoras, EPEAEK II / Researcher NKUA/ European Social Fund and National Resources / 7/2004-8/2006
- HPC- Europa Transnational Access programme / Research Visitor at Materials Science Center, Rijksuniversiteit Groningen, the Netherlands / EC / 10-11/2004
- Greek-Slovakian collaboration / Research Associate, NHRF / Greece-Slovakia funding / 9/2006-4/2008
- FP7-Capacities-Research Potential Of Convergence Regions / Research Associate, NHRF / EC / 5/2008-12/2011
- NATO Science For Peace And Security Programme / Research Associate, NHRF / NATO / 7/2009 – 7/2011
- ARISTEIA “COMANA” / Research Associate, Demokritos / National funding/ 3/2013 – 7/2014
- POLINANO, KRIPIS, ESPA / Research Associate, NHRF / European and National Funding / 8/2014 – 12/2015
- STSM grant / Visiting scientist, Physics Department, Universidade Nova de Lisboa, Lisbon, Portugal / EC / 4/2017
- Competitiveness, Entrepreneurship and Innovation, NSRF/ Research Associate, NHRF / European and National Funding / 12/2017-12/2018
- 12th Cy-Tera and Eastern Mediterranean HPC program / PI, NHRF / 12/2017-12/2018
- PNNL and TPCI/NHRF project / PI, NHRF / SPEC, PNNL / 3/2018-6/2019
- PNNL and Chemistry Department/NKUA project / PI, NKUA / SPEC, PNNL / 10/2019- 06/2020
- COST Action: CA17113 / Management Committee / EC / 10/2020-09/2022).
- COST Action: CA18212 / Management Committee / EC / 10/2020- 11/2023.
- PNNL and TPCI/NHRF project / PI, NHRF / SPEC, PNNL / 5/2022 - 8/2022
- COST Action: CA22131 / EC / 10/2023-10/2027

## REVIEWER OF SCIENTIFIC 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

## EDITOR OF BOOKS AND SPECIAL VOLUMES

Member of the Editorial Boards of the journals:

- E-Journal of Chemistry (impact factor 2016: 1.300, 2/2012-2/2017)
- International Journal of Computational and Theoretical Chemistry (2017-2020).
- The Open Physics Journal (2017-2019)
- The Open Access Journal of Science and Technology (2014- )
- Journal of Chemical Technology and Applications (2017- 2023)
- Molecules (impact factor: 4.927) (2020-2023)
  - 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
- Frontiers in Chemistry - Supramolecular Chemistry (Associate Editor, 2022-2024) (impact factor: 5.545)

## ADDITIONAL INFORMATION

- Presentations at conferences: **95**
- Supervision of doctoral theses: **4**
- Supervision of graduate students: **11**
- Supervision of undergraduate students: **6**
- PI in 6 Research Programs
- Collaboration/Participation in **20** Research Programs
- Reviewer in Research Programs: **>40** (Reviewer and Monitor for European Commission and for six Councils of European Countries)

## SELECTED PUBLICATIONS (link OF PUBLICATIONS)

### [Demeter Tzeli: Publications \(uoa.gr\)](http://uoag.gr)

1. Chalcogen Bonding and Hydrophobic Effects Force Molecules into Small Spaces  
F.-U. Rahman, D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, P. Ballester, J. Rebek Jr., Y. Yu, *J. Am. Chem. Soc.* **142**, 5876 (2020)
2. Quadruple Bonding in the Ground and Low-Lying Excited States of the Diatomic Molecules TcN, RuC, RhB, and PdBe, D. Tzeli, I. Karapetsas, *J. Phys. Chem. A* **124**, 6667 (2020).
3. The Effect of Geometry, Spin and Orbital Optimization in Achieving Accurate, Correlated Results for Iron-Sulfur Cubanes, C. Mejuto-Zaera, D. Tzeli, D. Williams-Young, N. M. Tubman, M. Matoušek, J. Brabec, L. Veis, S. S. Xantheas, W. A. de Jong, *J. Chem. Theory Comput.* **18**, 687-702 (2022)
4. 3-input AND molecular logic gate with enhanced fluorescence output: The key atom for the accurate prediction of the spectra, C. E. Tzeliou, D. Tzeli, *J. Chem. Inf. Model.* **62**, 6436 (2022)
5. Breaking Covalent Bonds in the Context of the Many-Body Expansion (MBE): I. The purported “first row anomaly” in  $XH_n$  ( $X = C, Si, Ge, Sn; n = 1-4$ ), D. Tzeli, S. S. Xantheas, *J. Chem. Phys.* **156**, 244303 (2022)
6. Analysis of chemical bonding of the ground and low-lying states of  $Mo_2$  and of  $Mo_2Cl_x$  complexes,  $x=2-10$ .” T. Depastas, A. Androutsopoulos, D. Tzeli *J. Chem. Phys.* **157**, 054302 (2022)
7. Magnetic anisotropy and structural flexibility in the field-induced single ion magnets  $[Co\{(OPPh_2)(EPPH_2)N\}_2]$ ,  $E = S, Se$ , explored by experimental and computational methods  
E. Ferentinos, D. Tzeli, S. Sottini, E. J. J. Groenen, M. Ozerov, G. Poneti, K. Kaniewska-Laskowska, J. Krzystek, P. Kyritsis, *Dalton Transactions* **52**, 2036 (2023)
8. Metallocene-naphthalimide derivatives: The effect of geometry, DFT methodology, and transition metals on absorption spectra, C.E. Tzeliou, D. Tzeli, *Molecules* **28**, 3565 (2023)
9. Photoswitchable Molecular Units with Tunable Non-Linear Optical Activity: A Theoretical Investigation  
A. Avramopoulos, H. Reis, D. Tzeli, R. Zalesny, M. G. Papadopoulos, *Molecules* **28**, 5646 (2023)
10. Microwave assisted, copper-catalyzed domino O-H/C-H arylation reaction towards the synthesis of oxygen-doped polyaromatic molecules, E. Kaplanai, E. Tonis, M. Drymona, Y. Zagranyski, D. Tzeli, G. C. Vougioukalakis, *J. Org. Chem.* **88**, 11552 (2023)
11. Computational and Spectroscopic analysis of the Quercetin encapsulation in  $(2HP-\beta-CD)_2$  and  $(2,6Me-\beta-CD)_2$  complexes, G. Leonis, V. Vakali, N. Zoupanou, N. Georgiou, D. A. Diamantis, A. G. Tzakos, T. Mauromoustakos, D. Tzeli, *J. Mol. Struct.* **1294**, 136430 (2023)
12. Electronic structure of low-lying states of triatomic  $MoS_2$  molecule. The building block of 2D  $MoS_2$   
M. A. Mermigki, I. Karapetsas, D. Tzeli, *Chem. Phys. Chem.* **24**, e202300365 (2023)
13. Hydration structure and dynamics, ultraviolet-visible and fluorescence spectra of caffeine in ambient liquid water. A combined classical molecular dynamics and quantum chemical study  
I. Skarmoutsos, D. Tzeli, I. D. Petsalakis, *J. Mol. Liquids* **391**, 123220 (2023)
14. Electronic Structure and Chemical Bonding of the First-, Second-, and Third-Row-Transition-Metal Monoborides: The Formation of Quadruple Bonds in RhB, RuB, and TcB  
C. Demetriou, C. E. Tzeliou, A. Androutsopoulos, D. Tzeli, *Molecules* **28**, 8016 (2023)