CURRICULUM VITAE

of

Zoi Salta

Personal Information

Name: Zoi **Surname:** Salta

Birthdate: 04/09/1981 **Birthplace:** Lamia, Greece

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Employment record

June 2018 - present: Research Associate

SMART Laboratory, Scuola Normale Superiore, Pisa, Italy.

Spring Semester 2018: Teaching assistant

"*Modern quantum and statistical mechanics techniques for the investigation of chemical reactions"*, Undergraduate course, Department of Chemistry, University of Ioannina, Greece.

Fall Semester 2017: Teaching assistant

"*Computational Chemistry Laboratory"*, Graduate course, Department of Chemistry, University of Ioannina, Greece.

Fall Semester 2008 – 2011: Teaching assistant

"*Physical Chemistry Laboratory 2: Electrochemistry, Chemical Kinetics and Physical Chemistry of Polymers*", Undergraduate course, Department of Chemistry, University of Ioannina, Greece.

Education

2014: Ph.D. in Chemistry:

Department of Chemistry, University of Ioannina, Greece.

Thesis: "Computational study of the peroxy nitroderivatives of methyl thiyl radical (CH_3S) – Structural, spectroscopic and energetic properties and modeling of their formation reactions in Atmospheric Chemistry."

2008: M.Sc. in Chemistry and Materials Science and Engineering:

Department of Chemistry, University of Ioannina, Greece.

Dissertation: "Computational study of structural, spectroscopic and thermodynamic properties of halogenated nitro-organic compounds and their formation-dissociation reaction pathways in the Atmosphere."

2005: B.Sc. in Materials Science and Engineering:

Department of Materials Science and Engineering, University of Ioannina, Greece.

Dissertation: "Computational study of structural, electronic and oscillatory properties of metallic nanowires of copper (Cu)."

Certified Foreign Languages

- German: Zertifikat, Goethe-Institut, 2004.
- English: Certificate of Proficiency in English, University of Cambridge, 1997.

Main Areas of Research

- Application of computational methodologies for gas-phase reactivity in astrochemical environments.
- Degradation processes in the natural environment with the use of hydrated clusters.
- Halogen bonded complexes and their use in biological systems.
- Quantum chemical applications in studies of molecular and thermodynamic properties of small molecules
- Kinetics and dynamics of heterogeneous chemical reactions in gas and aqueous phases – Theoretical calculations of rate constants.
- Spectroscopical studies and modeling of chemical behavior and reactivity of several chemical systems in gas phase.
- Radical reactions of atmospheric relevance.
- Molecular and electronic structure of ground and excited states.

Computer Skills

- *Simulation Package*s: Gaussian16, Materials Studio, XMD.
- *Molecular Visualization Programs:* GaussView, Hyperchem, Molden, VMD, XMakemol.

- *Other:* Experience with Ab Initio methods (DFT, HF, TB, MP2), Polarizable Continuum Model, Molecular Dynamics and NRL-Tight Binding Simulations, Parallel Computing Methods and Numerical Multidimensional Minimization Techniques.
- *Chemical kinetics programs:* Multiwell.

Fellowships and Awards

- Fellowship from the European Union (European Social Fund – ESF) and Greek national funds through the Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: **Heracleitus II**. Investing in knowledge society through the European Social Fund, Department of Chemistry, University of Ioannina, Greece, 2010-2013.
- Fellowship from the Bilateral Collaboration Program Greece-Slovenia, Ministry of Higher Education, Science and Technology of Slovenia – General Secretariat for Research and Technology of Greece, 2004-2007.

Participation in International and National Conferences

- 15th Eurasia Conference on Chemical Sciences, University of Sapienza, Rome, Italy, 5-8 September 2018. Oral presentation entitled: *"Computational Characterization of the Herbicide Metolachlor: Structure, Conformational Analysis and Monohydroxylated Photo Degradation Products."*.
- 5th Chemistry Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece, September 2017. Poster presentation entitled: *"Atmospheric degradation of the peroxy radical $CF_3OCH_2O_2$. A computational study of the reactions with HO_2 and NO."*.
- 5th Chemistry Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece, September 2017. Poster presentation entitled: *"Physicochemical and computational study of 3-Methyl-1,3-thiazolidine-2-thione complexes with dihalogens (I_2, IBr, ICl, BrBr, BrCl) for the design of novel drugs in thyroid disease treatments."*.
- 22nd Panhellenic Chemistry Conference Meeting, Thessaloniki, Greece, December 2016. Poster presentation entitled: *"Water complexes of halogenated nitromethanes. A*

computational study of structure and properties.”.

- International Conference of Computational Methods in Sciences and Engineering 2014 (ICCMSE 2014), Athens, Greece, April 2014. Oral presentation entitled: *“S-OO Bond Dissociation Energies and Enthalpies of Formation of the Thiomethyl Peroxyl Radicals $CH_3S(O)_nOO$ (n=0,1,2).”.*
- 12th Eurasia Conference on Chemical Sciences, Corfu, Greece, April 2012. Poster presentation entitled: *“Ab initio and DFT investigation of the structural and thermochemical properties of the peroxynitrates $CH_3S(O)_nOONO_2$ and the $CH_3S(O)_nOO$ decomposition radicals (n=0,1,2).”.*
- 14th International Density Functional Theory Conference - Applications in Physics, Chemistry, Biology, Pharmacy, Athens, Greece, September 2011. Poster presentation entitled: *“The atmospheric reactions between the alkylperoxy radicals RO_2 ($R=CH_3$, CH_3SCH_2 etc) and NO. Thermochemistry using DFT methods.”.*
- International Conference of Computational Methods in Sciences and Engineering 2007 (ICCMSE 2007), Corfu, Greece, September 2007.
- XX Panhellenic Conference on Solid State Physics & Materials Science, Ioannina, Greece, September 2004.
- 1st Panhellenic Symposium on «Porous Materials», Ioannina, Greece, March 2003.

Participation in Summer Schools

- International Series of Lectures entitled: «2004 Lectures in Chemistry and Physics» devoted to “The Nanotechnology Revolution”, FORTH, Heraclion Crete, Greece, July 2004.
- Summer School of “Advanced Materials”, National Center of Scientific Research “Demokritos”, Athens, Greece, July 2003.

Invited Lectures

- *“Computational Study of the Peroxyl Nitroderivatives of the Methylthiyl Radical (CH_3S)- Modeling of Formation Reactions in Atmospheric Chemistry”*, Graduate Conference Meeting, Department of Chemistry, University of Ioannina, Ioannina, Greece, March 2013.
- *Computational Study of the Formation of Halogenated N-organic Compounds and of Nitroderivatives of the Methylthiyl Radical (CH_3S) in the Atmosphere”*, Jožef Stefan Institute, Ljubljana, Slovenia, 18 November 2011.

Publications in Refereed Journals

- Kieninger, M., Salta, Z., Ventura, O.N., 2018. Theoretical determination of enthalpies of formation of benzyloxy, benzylperoxy, hydroxyphenyl radicals and related species in the reaction of toluene with the hydroxyl radical (to be submitted).
- Salta, Z., Segovia, M. E., Kosmas, A.M., Kieninger, M., Ventura, O.N., Barone, V., 2018. A reinvestigation of the deceptively simple reaction of toluene with $HO^{\bullet}$, and the fate of the benzyl radical. II. The "hidden" routes to cresols and benzaldehyde (to be submitted).
- Salta, Z., Segovia, M. E., Kosmas, A.M., Kieninger, M., Ventura, O.N., Barone, V., 2018. A reinvestigation of the deceptively simple reaction of toluene with $HO^{\bullet}$, and the fate of the benzyl radical. I. A combined thermodynamic and kinetic study on the competition between HO-addition and H-abstraction reactions. Journal of Physical Chemistry A (submitted).
- Salta, Z., Kosmas, A.M., Ventura, O.N., Barone, V., 2018. Computational evidence suggests that 1-chloroethanol may be an intermediate in the thermal decomposition of 2-chloroethanol into acetaldehyde and HCl. Journal of Physical Chemistry A (submitted).
- Petsis, G., Salta, Z., Kosmas, A.M., Ventura, O.N., 2018. Theoretical study of the microhydration of 1-chloro and 2-chloro ethanol as a clue for their relative propensity toward dehalogenation. International Journal of Quantum Chemistry (submitted).
- Salta, Z., Kosmas, A.M., Ventura, O.N., 2018. Kinetics and thermodynamics of the hydroxylation products in the photodegradation of the herbicide Metolachlor. Pure and Applied Chemistry (submitted).
- Salta, Z., Kosmas, A.M., Ventura, O.N., 2018. Computational characterization of the herbicide metolachlor and its mono-hydroxylated photodegradation products. Theoretical Chemistry Accounts 137:151. doi: 10.1007/s00214-018-2353-6.
- Salta, Z., Papayannis, D.K., Kosmas, A.M., 2017. Computational study of the hydrogen bonding interactions in the $[CH_2XNO_2 \cdot H_2O]$ clusters (X=H, F, Cl, Br, I). Computational and Theoretical Chemistry 1115, 63–68. doi: 10.1016/j.comptc.2017.05.028)
- Salta, Z., Kosmas, A.M., 2016. Computational investigation of the formation and isomerization pathways of CH_3SNO_2 and the S-N Bond Dissociation Energies of $CH_3S(O)_nNO_2$ (n=0,1,2). Struct. Chem. 27 (4), 1149–1156. doi: 10.1007/s11224-015-0737-y
- Salta, Z., Kosmas, A.M., Lesar, A., 2014. S-OO bond dissociation energies and enthalpies of

formation of the thiomethyl peroxyl radicals $CH_3S(O)nOO$ (n=0,1,2). AIP Conference Proceedings Series 1618, 916–919. doi: 10.1063/1.4897882

- Salta, Z., Kosmas, A.M., 2014. Computational study of the reaction of the methylsulfonyl radical, $CH_3S(O)_2$, with NO_2. International Journal of Quantum Chemistry 114, 1430–1437. doi: 10.1002/qua.24700
- Salta, Z., Kosmas, A.M., Lesar, A., 2012. Computational investigation of the peroxy radicals $CH_3S(O)_nOO$ and the peroxynitrates $CH_3S(O)_nOONO_2$ (n=0, 1, 2). Computational and Theoretical Chemistry 1001, 67–76. doi: 10.1016/j.comptc.2012.10.007
- Kosmas, A.M., Mpellos, C., Salta, Z., Drougas, E., 2010. Structural and heat of formation calculations of halogenated methyl hydro-peroxides. Chemical Physics 371, 36–42. doi: 10.1016/j.chemphys.2010.03.026
- Kosmas, A.M., Salta, Z., Lesar, A., 2009. Effect of halogenation on the mechanism of the atmospheric reactions between methylperoxy radicals and NO. A computational study. Journal of Physical Chemistry A 113, 3546–3554. doi: 10.1021/jp808895a
- Lesar, A., Salta, Z., Kovacic, S., Kosmas, A.M., 2007. Theoretical characterization of halogenated methylperoxy nitrites $CX_nY_{3-n}OONO$ (X, Y=H, F, Cl). Chemical Physics Letters 446, 268–275. doi:10.1016/j.cplett.2007.08.062