

CURRICULUM VITAE

Athanassios CHRISSANTHOPOULOS

*Chemist (PhD in Chemical Engineering), Lecturer of Inorganic Chemistry –
Computational Chemistry*

Address: Laboratory of Inorganic Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, University campus, Zografou 157 84, Greece, tel. +30 210 7274218, e-mail: achryssan@chem.uoa.gr

PROFESSIONAL EXPERIENCE

17/1/2014-today: Lecturer, Department of Chemistry, National and Kapodistrian University of Athens.

2001-2013: Lecturer and/or Assistant professor (under contract, ΠΔ 407/1980), Departments of Chemistry, Materials Science and Pharmacy, University of Patras.

RESEARCH ACTIVITIES

- *Nanoscience/nanotechnology:* Synthesis of inorganic (mainly ZnO and ZnO/C hybrid) nanostructured materials and characterization using light scattering, light absorbance, photoluminescence and microscopy techniques, having as a final goal to understand the nanostructure growth mechanism and to control their physicochemical/optical properties.
- *Computational chemistry:* Structural, vibrational properties and molecular interactions using abinitio, DFT and/or semiempirical molecular orbital theoretical/computational methods.
- *Raman spectroscopy:* Investigation of the structure/structural changes of inorganic materials in solid (crystalline, glassy) and liquid state.
- *f-f hypersensitive transitions as a rare earth halides' structural probe.*

TEACHING ACTIVITIES

2014-today: Inorganic chemistry and Spectroscopy laboratory courses at the Departments of Biology and Chemistry (National and Kapodistrian University of Athens).

2001-2013: Physical Chemistry, Inorganic and Chemical Analysis courses at the Departments of Chemistry, Materials Science and Pharmacy (University of Patras). Co-advisor of more than 12 undergraduate diploma Theses.

HONORS/AWARDS

- Outstanding Undergraduate Student Excellence Awards
- **FORTH-ICE/HT** Fellowship for Ph.D. studies
- **NATO** fellowships for attending NATO-ASI school
- **EU** fellowships for short period visit and collaboration at CNRS, Orleans
- **ESF** (European Science Foundation) fellowship for post-doctoral research training in the area of Femtochemistry and Femtobiology (Germany).

- **DAAD** (Deutscher Akademischer Austauschdienst) three months fellowship for post-doctoral research training (Germany).

REVIEWING

1. Journal of Chemical Physics (American Institute of Physics).
2. Journal of Physics and Chemistry of Solids (Elsevier).
3. Thin Solid Films (Conference volume) (Elsevier).
4. Electrochemical and Solid-State Letters (ESL) (The Electrochemical Society).
5. Current Applied Physics (Elsevier).
6. Vibrational Spectroscopy (Elsevier).
7. Current Nanoscience (Bentham).
8. Materials Letters (Elsevier).
9. Physica E (Elsevier).
10. Nanoscale Research Letters (Springer).
11. Materials (open journal, MDPI).
12. Journal of Nanostructured Polymers and Nanocomposites.
13. Materials Science in Semiconductor Processing (Elsevier).
14. Materials Science and Engineering B (Elsevier).
15. Journal of Materials Science (Springer).
16. CrystEngComm (Royal Society of Chemistry)

VISITING SCIENTIST at the:

- Institute of Chemical Engineering and High-Temperature Chemical Processes (FORTH/ICE-HT) (collaboration with Prof. G.N. Papatheodorou and Dr. S.N. Yannopoulos).
- 21/1/2001-12/2/2001 & 1/6/2001-1/9/2001: Laboratoire de Chimie Structurale Universite de Pau et des Pays de l' Adour (collaboration with Prof. C. Pouchan).
- 01/04/1999-30/06/1999 & 01/11/2000-30/11/2000: Institute of Theoretical and Physical Chemistry, Technical University of Braunschweig, Germany (collaboration with Prof. U. Hohm).
- 01/2000–today: Prof. G. Maroulis Computational Chemistry research group, Department of Chemistry, Patras, Greece.
- 13/09/1998-18/09/1998: Daresbury Laboratory Synchrotron Radiation Source, Warrington, United Kingdom (collaboration with Sabyasachi Sen -Associate Professor, Dept. of Chemical Eng. & Materials Science, University of California, Davis- and Dr. G.D. Zissi, Dept. of Pharmacy, Univ. of Patras).
- High Resolution Solid and High Temperature Liquid Multinuclear NMR at CRMHT-Orléans France (collaboration with Dr. Frank Fayon).

PUBLICATIONS IN REFEREED JOURNALS

- 44. Inhibition of Hydroxyapatite Formation in the presence of Titanocene-aminoacid complexes; an experimental and computational study**, A. Chrissanthopoulos, N. Klouras, Ch. Ntala, D. Sevastos, E. Dalas, *J Mater Sci: Mater Med* 21 (2014) submitted.
- 43. The influence of Au film thickness and annealing conditions on the VLS-assisted growth of ZnO nanostructures**, K. Govatsi, A. Chrissanthopoulos, V. Dracopoulos, S.N. Yannopoulos, *Nanotechnology* (2014) submitted.
- 42. ZnO/zeolite hybrid nanostructures: synthesis, structure, optical properties and simulation**, A. Chrissanthopoulos, F.C. Kyriazis, V. Nikolakis, I.G. Giannakopoulos, V. Dracopoulos, S. Baskoutas, N. Bouropoulos, S. N. Yannopoulos, *Thin Solid Films* 555 (2014) 21–27.
- 41. Influence of thermal history on the photostructural changes in glassy As₁₅S₈₅ studied by Raman scattering and ab initio calculations**, J. Kolar, L. Strizik, T. Kohoutek, T. Wagner, G. A. Voyiatzis, A. Chrissanthopoulos, S. N. Yannopoulos, *J. Appl. Phys.* 114(20), (2013) 203502 - 203502-7 (<http://dx.doi.org/10.1063/1.4832830>).
- 40. Stability and physicochemical characterization of novel milk-based oral formulations**, J. Kytariolos, G. Charkoftaki, J.R. Smith, G. Voyiatzis, A. Chrissanthopoulos, S.N. Yannopoulos, D.G. Fatouros, P. Macheras, *International Journal of Pharmaceutics* 444 (2013) 128–138.
- 39. Structure of AgI-doped Ge-In-S glasses: Experiment, reverse Monte Carlo modelling, and density functional calculations**, A. Chrissanthopoulos, P. J v ari, I. Kaban, S. Gruner, T.Kavetsky, J.Borc, W. Wang, J. Ren, G. Chen, S.N. Yannopoulos, *Journal of Solid State Chemistry* 192 (2012) 7.
- 38. Silicate Glasses at the Ionic Limit: Alkaline-Earth Sub-Orthosilicates**, N. K. Nasikas, A. Chrissanthopoulos, N. Bouropoulos, S. Sen, G.N. Papatheodorou, *Chem. Mater.* 2011, 23, 3692–3697 (dx.doi.org/10.1021/cm2012582).
- 37. Enhanced Raman gain of Ge-Ga-Sb-S chalcogenide glass for highly nonlinear microstructured optical fibers**, Tomas Kohoutek, Xin Yan, Teruo Shiosaka, Spyros Yannopoulos, Athanassios Chrissanthopoulos, Takenobu Suzuki, and Yasutake Ohishi, *J. Opt. Soc. Am. B / Vol.* 28, No. 9 / September 2011.
- 36. Vibrational dynamics and surface structure of amorphous materials**. T. Scopigno, W. Steurer, S. N. Yannopoulos, A. Chrissanthopoulos, M. Krisch, G. Ruocco and T. Wagner, *Nature Communications* (2011), 2:195, Febr. 2011.
- 35. Structure and vibrational modes of AgI-doped AsSe glasses: Raman scattering and ab-initio calculations**, O. Kostadinova, A. Chrissanthopoulos, T. Petkova, P. Petkov and S.N. Yannopoulos, *Journal of Solid State Chemistry* 184 (2), (2011) 447-454.
- 34. Synthesis and characterization of ZnO/NiO p-n heterojunctions: ZnO nanorods grown on NiO thin film by thermal evaporation**. A. Chrissanthopoulos, S. Baskoutas, N. Bouropoulos, V. Dracopoulos, P. Pouloupoulos and S. N. Yannopoulos, *Photonics and Nanostructures* (2011), Volume 9, Issue 2, April 2011, Pages 132-139.
- 33. Novel composites materials from functionalized polymers and silver coated titanium oxide capable for calcium phosphate induction, control of Orthopedic biofilm infections. An “in vitro” study**. Minos Tyllianakis, Evangelos Dalas, Myrto Christofidou, Joannis Kallitsis, Athanassios Chrissanthopoulos, Petros G. Koutsoukos, Christina Bartzavali, Nora Gourdoupi, Konstantinia Papadimitriou, Eudokia K. Oikonomou, Spyros N. Yannopoulos; *J Mater Sci: Mater Med* 21 (2010) 2201–2211.
- 32. Effect of silver doping on the structure and phase separation of sulfur-rich As-S glasses: Raman and SEM studies**, F. Kyriazis, A. Chrissanthopoulos, V. Dracopoulos, M. Krbal, T. Wagner, M. Frumar, and S.N. Yannopoulos, *J. Non-Cryst. Solids*, 355 (2009) 2010–2014.

- 31. The Ho(III) as structural probe for high temperature ionic liquids: RCl₃ (R= rare earth),** A. Chrissanthopoulos, G.N. Papatheodorou, *J. Mol. Struct.* **892** (2008) 93–102.
- 30. A Density Functional Investigation of the Structural and Vibrational properties of the highly symmetric molecules M₄O₆, M₄O₁₀ (M= P, As, Sb, Bi),** A. Chrissanthopoulos and C. Pouchan, *Vibrational Spectroscopy* **48** (2008) 135–141.
- 29. Optical and Dielectric Properties of ZnO/PVA Nanocomposites,** N. Bouropoulos, G.C. Psarras, N. Moustakas, A. Chrissanthopoulos and S. Baskoutas, *Physica Status Solidi (a)* **205** No. 8 (2008) 2033–2037.
- 28. Effect of cluster size of chalcogenide glass nanocolloidal solutions on the surface morphology of spin-coated amorphous films,** T. Kohoutek, T. Wagner, M. Frumar, A. Chrissanthopoulos, O. Kostadinova, S.N. Yannopoulos, *J. Appl. Phys.* **103** (2008) 063511.
- 27. Vibrational spectroscopic and computational studies of sol-gel derived CaO-MgO-SiO₂ binary and ternary bioactive glasses,** A. Chrissanthopoulos, N. Bouropoulos and S.N. Yannopoulos, *Vibrational Spectroscopy* **48** (2008) 118–125.
- 26. Preparation of ZnO nanoparticles by thermal decomposition of zinc alginate,** S. Baskoutas, P. Giabouranis, S. Yannopoulos, V. Dracopoulos, L. Toth, A. Chrissanthopoulos, N. Bouropoulos, (2007), *Thin Solid Films* (2007), **515** (2007) 8461–8464.
- 25. Novel ZnO nanostructures grown on carbon nanotubes by thermal evaporation,** A. Chrissanthopoulos, S. Baskoutas, N. Bouropoulos, V. Dracopoulos, D. Tasis and S. N. Yannopoulos, *Thin Solid Films*, **515** (2007) 8524–8528.
- 24. Semiempirical Molecular Orbital Study of Glycine solvation and of Binding Calcium Carbonate on Glycine polypeptides,** A. Chrissanthopoulos, E. Dalas, *Journal of Computational Methods in Sciences and Engineering*, **7** (2007) 75-84.
- 23. Calcite particles formation, in the presence of soluble polyvinyl-alcohol matrix,** P. Malkaj, E. Dalas, D.G. Kanellopoulou, A. Chrissanthopoulos, D. Sevastos, *Powder Technology*, **177** (2007) 71–76.
- 22. Vapor complexation in the CsI-HoI₃ system up to 1300 K and the f ← f hypersensitive transition intensities of Ho(III) in different coordination geometries,** G.N. Papatheodorou, A. Chrissanthopoulos, *J. Mol. Struct.* **832**(1-3), (2007) 38-47.
- 21. Crystallization of Hydroxyapatite on Oxadiazole-Based Homopolymers.** J. Kanakis, A. Chrissanthopoulos, N. P. Tzanetos, J. K. Kallitsis, and E. Dalas, *Crystal Growth & Design* (2006), **6** (6), 1547–1552.
- 20. Calcium phosphate crystallization on polyglycine, polytyrosine and polymethionine.** A. Chrissanthopoulos, P. Malkaj, E. Dalas, *Materials Letters* (2006), 3874-3878.
- 19. ZnS deposition on oxadiazole-terpyridine copolymer.** A. Chrissanthopoulos, N.P. Tzanetos, A.K. Adreopoulou, J. Kallitsis, E. Dalas, *J. Appl. Polym. Sci.* (2006), **101** (3), 1913-1918.
- 18. Vibrational modes and structure of the LaCl₃-CsCl melts.** Zissi, G.D.; Chrissanthopoulos, A.; Papatheodorou, G.N., *Vibrational Spectroscopy* (2006), **40** (1), 110-117.
- 17. Temperature dependence of the f ← f hypersensitive transitions of Ho³⁺ and Nd³⁺ in molten salt solvents and the structure of the LaCl₃-KCl melts.** A. Chrissanthopoulos and G.N. Papatheodorou, *Journal of Molec. Struct.* (2006), **782** (2-3), 130-142.
- 16. The structure of molten rare earth iodide-alkali iodide mixtures.** A. Chrissanthopoulos, G.D. Zissi and G.N. Papatheodorou, *Zeitschrift fuer Naturforschung, A: Physical Sciences* (2005), **60** (10), 739-748.
- 15. Calcite crystallization on oxadiazole-terpyridine copolymer.** Chrissanthopoulos, A.; Tzanetos, N.P.; Adreopoulou, A.K.; Kallitsis, J.; Dalas, E., *Journal of Crystal Growth* (2005), **280** (3-4), 594-601.

- 14. Numerical investigation of methane combustion under mixed air-steam turbine conditions-FLAMESEEK.** Skevis, G.; Chrissanthopoulos, A.; Goussis, D. A.; Mastorakos, E.; Derksen, M. A. F.; Kok, J. B. W., *Applied Thermal Engineering* (2004), **24** (11-12), 1607-1618.
- 13. Understanding nucleation of calcium carbonate on gallium oxide using computer simulation.** Malkaj, P.; Chrissanthopoulos, A.; Dalas, E.; *Journal of Crystal Growth* (2004), **264** (1-3), 430-437.
- 12. The overgrowth of hydroxyapatite on new functionalized polymers.** Dalas, E.; Chrissanthopoulos, A., *Journal of Crystal Growth* (2003), **255** (1-2), 163-169.
- 11. Calcite overgrowth on carboxylated polymers.** Dousi, E.; Kallitsis, J.; Chrissanthopoulos, A.; Mangood, A. H.; Dalas, E., *Journal of Crystal Growth* (2003), **253** (1-4), 496-503.
- 10. Temperature induced changes on the structure and the dynamics of the "tetrahedral" glasses and melts of ZnCl₂ and ZnBr₂.** Yannopoulos, S. N.; Kalampounias, A. G.; Chrissanthopoulos, A.; Papatheodorou, G. N.; *Journal of Chemical Physics* (2003), **118**(7), 3197-3214.
- 9. The overgrowth of calcium carbonate hexahydrate on new functionalized polymers.** Malkaj, P.; Chrissanthopoulos, A.; Dalas, E.; *Journal of Crystal Growth* (2002), **242** (1-2), 233-238.
- 8. Structural investigation of vanadium - sodium metaphosphate glasses.** Chrissanthopoulos, A.; Pouchan, C.; Papatheodorou, G. N.; *Zeitschrift fuer Naturforschung, A: Physical Sciences* (2001), **56** (11), 773-776.
- 7. Structure of Vanadium Oxosulfato Complexes in V₂O₅-M₂S₂O₇-M₂SO₄ (M = K, Cs) Melts. A High Temperature Spectroscopic Study.** Boghosian, Soghomon; Chrissanthopoulos, Athanassios; Fehrmann, Rasmus. *Journal of Physical Chemistry B* (2002), **106** (1), 49-56.
- 6. Thermophysical properties of tetramethylmethane and tetramethylsilane gas calculated by means of an isotropic temperature-dependent potential.** Zarkova, L.; Pirgov, P.; Hohm, U.; Chrissanthopoulos, A.; Stefanov, B. B.; *International Journal of Thermophysics* (2000), **21** (6), 1439-1461.
- 5. Electric dipole moment and polarizability of ScF.** Chrissanthopoulos, Athanassios; Maroulis, George; *Journal of Physics B: Atomic, Molecular and Optical Physics* (2001), **34** (1), 121-125.
- 4. Probing the structure of GdCl₃-KCl melt mixtures by electronic absorption spectroscopy of the hypersensitive f←f transitions of Ho³⁺ and by Raman spectroscopy.** Chrissanthopoulos, A.; Papatheodorou, G. N.; *Physical Chemistry Chemical Physics* (2000), **2**(16), 3709-3714.
- 3. Frequency-dependence of the polarizability anisotropy of CO₂ revisited.** Chrissanthopoulos, A.; Hohm, U.; Wachsmuth, U.; *Journal of Molecular Structure* (2000), **526**, 323-328.
- 2. Vanadium(V) complexes in molten salts of interest for the catalytic oxidation of sulfur dioxide.** Boghosian, Soghomon; Borup, Flemming; Chrissanthopoulos, Athanassios; *Catalysis Letters* (1997), **48**(3,4), 145-150.
- 1. Catalytic activity and deactivation of SO₂ oxidation catalysts in simulated power plant flue gases.** Masters, S. G.; Chrissanthopoulos, A.; Erikson, K. M.; Boghosian, S.; Fehrmann, R.; *Journal of Catalysis* (1997), **166** (1), 16-24.

BOOK CHAPTERS:

- 1.** Ofeliya Kostadinova, T. Petkova, A. Chrissanthopoulos, Plamen Petkov, and S. N. Yannopoulos, 'Structure of AgI-AsSe Glasses by Raman Scattering and Ab Initio Calculations', chapter 23 in J. P. Reithmaier et al. (eds.), *Nanotechnological Basis for Advanced Sensors NATO Science for Peace and Security Series B: Physics and Biophysics* 2011, pp 217-223.
- 2.** T. Kohoutek, T. Wagner, M. Frumar, A. Chrissanthopoulos, O. Kostadinova, S. N. Yannopoulos, "Nanocolloidal solutions of As-S glasses and their relation to the surface morphology of spin-

coated amorphous films", in NATO Science for Peace and Security Series B: Physics and Biophysics (Nanostructured Materials for Advanced Technological Applications), Springer, (2009), pp. 361-364.

3. F. Kyriazis, S. N. Yannopoulos, A. Chrissanthopoulos, S. Baskoutas, N. Bouropoulos, "ZnO nanostructures grown by thermal evaporation and thermal decomposition methods", in NATO Science for Peace and Security Series B: Physics and Biophysics (Nanostructured Materials for Advanced Technological Applications), Springer, (2009), pp. 211-214.

4. A. Chrissanthopoulos and D. Tasis, "DFT studies about the interaction of carbon nanotubes with various chemical species", Review chapter in the book "DFT calculations on fullerenes and carbon nanotubes" (edited by V.A. Basiuk and S. Irlle), The Research Signpost, in print (2008).

5. A. Chrissanthopoulos and G.N. Papatheodorou, "The electronic hypersensitive transitions as structural probe for molten rare-earth trichlorides", in Progress in Molten Salts Chemistry 1 (edited by R.W. Berg and H.A. Hjuler), Elsevier Paris (2000) 167-171 (ISBN 2-84299-249-0).

REFERRED PUBLICATIONS IN INTERNATIONAL CONFERENCE PROCEEDINGS:

13. Computer simulation study of low dimensional structures of As-S glasses, A. Chrissanthopoulos, F. Kyriazis and S.N. Yannopoulos, International Conference on Computational Methods in Sciences and Engineering 2008 (ICCMSE 2008), (edited by: George Maroulis, Theodore E. Simos), AIP Conference Proceedings 1148, ISBN 978-0-7354-0685-8

12. Semiempirical Molecular Orbital Study of Binding of Calcium Carbonate on Polypeptides, A. Chrissanthopoulos and E. Dalas, Lecture Series on Computer and Computational Sciences (2006), (International Conference of Computational Methods in Sciences and Engineering 2006), vol. **7B** 1459-1462.

11. Electric properties of boron and aluminum trihalides. Chrissanthopoulos, A.; Maroulis, G., Lecture Series on Computer and Computational Sciences (2004), 1(International Conference of Computational Methods in Sciences and Engineering 2004), 1065-1068.

10. UV/Vis spectroscopic investigation of the vapor species above HoI_3 and CsI.HoI_4 . Chrissanthopoulos, A.; Zissi, G. D.; Papatheodorou, G. N., Institute of Physics Conference Series (2004), **182** (Light Sources 2004), 269-270.

9. Structural investigation of the caesium-lanthanide(III) iodide melts using Raman spectroscopy. Chrissanthopoulos, A.; Zissi, G. D.; Papatheodorou, G. N., Institute of Physics Conference Series (2004), **182** (Light Sources 2004), 267-268.

8. Physicochemical Properties of Lanthanide(III) Iodide Species Formed In and Above Molten Salts, A. Chrissanthopoulos, G. D. Zissi and G. N. Papatheodorou; Proceedings - Electrochemical Society **PV 2004-24** Molten Salts XIV, (2004) 825.

7. Analysis of Methane-Air Flame Structures near Extinction Limits Using CSP, A. Chrissanthopoulos, G. Skevis and E. Mastorakos, 4th GRACM congress on computational mechanics Proceedings, Patras, (2002).

6. The electronic hypersensitive transitions as structural probe for molten rare-earth trichlorides, A. Chrissanthopoulos and G.N. Papatheodorou, in Progress in Molten Salts Chemistry 1, Elsevier Paris (2000) 167-171 (ISBN 2-84299-249-0).

5. Molten rare earth halides: Structure and thermodynamics. Chrissanthopoulos, A.; Zissi, G. D.; Papatheodorou, G. N.; Schriften des Forschungszentrums Juelich, Reihe Energietechnik/Energy Technology (2000), 15 (Pt. 1, High Temperature Materials Chemistry, Part 1), 43-48.

4. Structural and redox properties of vanadium complexes in molten salts of interest for the catalytic oxidation of sulfur dioxide. Boghosian, Soghomon; Chrissanthopoulos, Athanassios; Fehrmann, Rasmus; Proceedings - Electrochemical Society (2000), 99-41(Molten Salts XII), 228-239.

3. Activity and deactivation of molten salt catalysts during SO_2 oxidation and flue gas

desulfurization. Chrissanthopoulos, A.; Masters, S. G.; Zervopoulou, E.; Psarakis, P.; Boghosian, S.; Environmental Research Forum (1996), 1-2(Chemistry and Energy), 55-61.

2. Physicochemical and structural properties of DeNO_x and SO₂ oxidation catalysts. Masters, S. G.; Oehlers, C.; Nielsen, K.; Eriksen, K. M.; Fehrmann, R.; Chrissanthopoulos, A.; Boghosian, S.; Proceedings - Electrochemical Society (1996), 96-7(Molten Salts), 74-79.

1. Activity and deactivation of molten salt catalyst during SO₂ oxidation and SO₂ removal from flue gasses. Boghosian, S.; Chrissanthopoulos, A.; Karydis, D. A.; Masters, S. G.; Eriksen, K. M.; Fehrmann, R.; Proceedings - Electrochemical Society (1994), 94-13(MOLTEN SALTS), 625-32.

INTERNATIONAL CONFERENCES' PRESENTATIONS (oral or poster): 43

Web of science citation report (12/4/2014)

Results found:	42
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