GEORGIOS S. FANOURGAKIS

Curriculum vitae

December 2022

Laboratory of Quantum and Computational Chemistry,
School of Chemistry,
Aristotle University of Thessaloniki

Georgios S. Fanourgakis

Current Professional Employment

Address: Laboratory of Quantum and Computational Chemistry, School of Chemistry, Aristotle University of Thessaloniki (AUTH) University Campus, GR-54124, Thessaloniki, Greece

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Position: Assistant Professor

Personal information

Place and date of birth: Athens, 8 February 1969

Nationality: Greek citizen

Obligatory Military service : May 1998 – January 2000

ORCID: 0000-0001-6158-6824

Researcher ID: ABH-3162-2021

Education

September 1995 - December 1999 — Chemistry Department, University of Crete

Doctorate (Ph.D.) in Theoretical and Computational Chemistry. Thesis title: **"Study of ionic clusters of the form: X^+L_n. Application to Mg^+Ar_n, Sr^+Ar_n clusters"**
Advisor Prof. S. C. Farantos

September 1992 - June 1994 — Chemistry Department, University of Crete

Master (M.Sc.) in Theoretical and Computational Chemistry. Thesis title: **"Study of static and dynamic properties of the $Mg^{+(+)}Ar_n$ clusters"**
Advisor Prof. S. C. Farantos

September 1987 - September 1991 — Physics Department, University of Crete

B.Sc. diploma in physics

Professional Employment

May 2018 - December 2022 — UoC, Greece
Research Associate
Materials Modeling and Design Group (MMDG)
University of Crete, Department: Chemistry, Heraklion, Greece
Research Director: G. Froudakis

October 2013 - April 2018 — UoC, Greece
Research Associate
Environmental Chemical Processes Laboratory
University of Crete, Department: Chemistry, Heraklion, Greece
Research Director: M. Kanakidou

January 2012 - September 2013 — CaSToRC, CyI, Cyprus
Research Associate
Cyprus Institute (CyI) Department: (CaSToRC) Nicosia, Cyprus

September 2010 - January 2012 — CSIC
PostDoctoral Fellow — Spain
Spanish National Research Council (CSIS), Instituto de Física Fundamental (IFF) Department: Física Atómica, Molecular y Agregados Madrid, Spain
Research Advisor: R. Prosmiti

September 2007 - August 2010 — IESL, FORTH
Research Scientist — Greece
Institute for Electronic Structure and Laser, Foundation for Research and Technology Hellas, GR71110, Heraklion, Greece
Under a Personal European Marie Curie Grant

July 2003 - July 2007 — PNNL
Postdoctoral Fellow — USA
Molecular Interactions and Transformations, Chemical and Materials Sciences Division, Pacific Northwest National Laboratory (PNNL) Richland, Washington USA
Research Advisor: S. S. Xantheas

February 2002 - May 2003 — UWO
Postdoctoral Fellow — Canada
University of Western Ontario, London, Ontario, Canada
Research Advisor: S. Consta

February 2000 - February 2002 — Cecam
Postdoctoral Fellow — France
Centre Européen de Calcul Atomique et Moléculaire (CECAM) Lyon, France
Research Advisor: V. Pontikis

Scholarships - Research Grants

September 2007 - August 2010
Marie Curie International Re-integration Grant (IRG)
SIMULAQI ("Simulations of aqueous interfaces")

November 2007 - December 2007
Financial support from the "HPC-Europa Transnational Access Programme" to visit Edinburgh Parallel Computing Centre (EPCC) (1 week) and Prof. D. Manolopoulos, Department of Chemistry, Oxford University (3 weeks)

July 2003 - July 2007
Postdoctoral fellowship (PNNL, USA)

February 2002 - May 2003
Postdoctoral fellowship (UWO, Canada)

February 2000 - February 2002
Postdoctoral fellowship (CECAM, France)

March 1996 - September 1996
Financial support from "ERASMUS" Program to visit Laboratoire de PhotoPhysique Moléculaire, Université Paris SUD, Orsay, FRANCE. *Research Advisors:* Prof. P. Parneix and Prof. Ph. Bréchignac.

September 1992 - May 1998

Successive full scholarships, awarded by the Department of Chemistry, University of Crete and the Institute of Electronic Structure and Laser (IESL), Foundation for Research and Technology – Hellas (FORTH)

Teaching Experience

March 2012 - October 2022 — Dept. of Chemistry, Univ. of Crete

Responsible for certain lectures in Physics (classical mechanichs), atmospheric chemistry, Introduction to programming

September 2011 - February 2012 — Dept. of Materials Science and Technology, Univ. of Crete

Teaching of Statistical Thermodynamics

September 2010 - February 2011 — Dept. of Materials Science and Technology, Univ. of Crete

Teaching of Statistical Thermodynamics

September 2009 - February 2010 — Dept. of Materials Science and Technology, Univ. of Crete

Teaching of Statistical Thermodynamics

February 2008 - June 2008 — Dept. of Chemistry, Univ. of Crete

Teaching of Physics I (Classical Mechanics)

September 1992 - May 1999 — Dept. of Chemistry, Univ. of Crete

Responsible for certain lectures and exams evaluation

Scientific techniques & Skills

Statistical mechanics methods

- Classical Molecular Dynamics simulation techniques
- Classical Monte-Carlo simulation techniques
- Quantum (path integral) Centroid Molecular Dynamics simulation techniques

Machine Learning methods

Application of Machine learning techniques (e.g. Random Forest, Gaussian Processes, Neural Networks) in physical chemistry related problems, such as

- Prediction of gas adsorption of nanoporous materials
- Development of ab-initio based force fields for water

First principles (ab-initio) methods

- Correlated methods for ground and excited states of atomic and molecular clusters
- LDA/DFT methods for solids

Development and Applications

- Development of parallel classical and quantum (Path Integral) Molecular Dynamics and Monte-Carlo codes

- Development of force fields describing intermolecular interactions from first principle electronic structure calculations

- Study of the solid and liquid phases of small ionic clusters and bulk water using classical and quantum Molecular Dynamics and Monte-Carlo methods

- Development of theoretical methods for ordinary differential equations and application to atmospheric chemistry problems

- Study of the influence of hydrostatic pressure on the materials

Computer Skills

- Fortran-77/90/95 and C on AIX, Linux and Windows environments

- Parallel programming using the Global Arrays (GA) toolkit, the Message Passing Interface (MPI) and the openMP. Knowledge on general purpose GPU programming

- Development of applications in Python

- Knowledge of NetCDF3/4 and HDF4/5

- Experience in using Data Visualization and Analysis packages (i.e. Ferret)

- Experience in developing scientific parallel codes for shared- and distributed-memory computer platforms. Participation to the PRACE winter school (Athens, 10-13 Feb. 2009)

Invited talks in Foreign Institutes

12-23 September 2011
Max Planck Institute for Chemistry, Mainz, Germany (Collaboration with Prof. J. Lelieveld)

4 July 2011
CaSToRC, The Cyprus Institute, Nicosia, Cyprus
"Molecular Simulations: Challenges and opportunities" *(Invited talk)*

20-29 June 2009
Institute of fundamental physics, Department of atomic, molecular and cluster physics, Madrid, Spain
"Development of ab initio based water models and quantum molecular simulations of liquid water" *(Invited talk)*

12 November - 5 December 2007
Physical and Theoretical Chemistry Laboratory, Oxford, UK (Collaboration with Prof. Manolopoulos)

October 2003 - February 2004
Department of Chemistry, University of Kaiserslautern, Kaiserslautern, Germany
"Structure and stability of $(H_2O)_{20}$. High level ab-initio results and comparison with empirical force fields" *(Invited talk)*

15-20 May 2003
Pacific Northwest National Laboratory (PNNL), Richland, WA, USA
"I. Influence of the hydrostatic pressure on Aluminum crystal. Study using classical potentials and ab initio methods" and "II. A spectroscopic and computer simulation study of butanol vapors" *(Invited talk)*

15 March -12 April 1998
Pacific Northwest National Laboratory (PNNL), Richland, WA, USA
"Photo fragmentation spectra and structures of Sr^+Ar_n, $n = 2 - 8$ clusters: Experiment and theory" *(Invited talk)*

March 1996 - September 1996

Laboratoire de PhotoPhysique Moléculaire, Université Paris SUD, Orsay, France.
"An effective transition state theory for the isomerization of the Mg^+Ar_{12} cluster" *(Invited talk)*

International Workshops

6-8 March 2013 — PRACE WP8 face-to-face meeting
Swiss national supercomputing center (CSCS) — Lugano, Switzerland

11-13 June 2012 — PRACE WP8 face-to-face meeting
"Maison de la Simulation" Paris-Saclay, — Paris, France

2-3 February 2012 — PRACE WP8 face-to-face meeting
Barcelona super computing center (BSC) — Barcelona, Spain

18 October 2011 — PRACE WP8 face-to-face meeting
Swiss national supercomputing center (CSCS) — Lugano, Switzerland

Participation in Workshops / Schools

28-31 May 2014

Participation at the 12th International "Conference on Meteorology, Climatology and Atmospheric Physics" (COMECAP) that took place in Hereklion, Crete

19-21 February 2013

Participation in the "Third LinkSCEEM Thematic Workshop for Climate Research" held at the Computation-based Science and Technology Research Center (CaSToRC) of the Cyprus Institute, Nicosia, Cyprus.

12 December 2012

Participation in the "LinkSCEEM/Cy-Tera GPU Workshop" held at the Computation-based Science and Technology Research Center (CaSToRC) of the Cyprus Institute, Nicosia, Cyprus.

11-13 October 2011

Participation in the "1^{st} LinkSCEEM thematic workshop for Climate Research" held at the Computation-based Science and Technology Research Center (CaSToRC) of the Cyprus Institute, Nicosia, Cyprus.

10-13 February 2009

Participation in the "PRACE workshoa:Principles of parallel programming and computer models" held in Athens, Greece.

3-28 July 1995

Participation in the Summer School "Monte Carlo and Molecular Dynamics of Condensed Matter Systems", Como, Italy

Publications in Peer-reviewed Scientific Journals

1. **G. S. Fanourgakis** and S. C. Farantos, "Potential functions and static and dynamic properties of $Mg^{m+}Ar_n$ $(m = 1, 2; n = 1 - 18)$ clusters", *Journal of Physical Chemistry*, **100**, 3900 (1996)
2. **G. S. Fanourgakis**, S. C. Farantos, P. Parneix and Ph. Bréchignac, "An effective transition state for a complex cluster isomerization process: Comparison between anharmonic and harmonic models for Mg^+Ar_{12}", *Journal of Chemical Physics* **106**, 4954 (1997)

3. J. Papadakis, **G. S. Fanourgakis**, S. C. Farantos, M. Founargiotakis, "Comparison of line search minimization algorithms for exploring topography of multidimensional potential energy surfaces: Mg^+Ar_n case", *Journal of Computational Chemistry* **18**, 1011, (1997)
4. S. S. Xantheas, **G. S. Fanourgakis**, S. C. Farantos and M. Velegrakis, "Spectroscopic constants of the $X^2\Sigma^+$ and $A^2\Pi$ states of Sr^+Ar from first principles: Comparison with experiment", *Journal of Chemical Physics* **108**, 46 (1998)
5. **G. S. Fanourgakis**, S. C. Farantos, Ch. Lüder, M. Velegrakis and S. S. Xantheas, "Photofragmentation spectra and structures of Sr^+Ar_n, $n = 2 - 8$ clusters: Experiment and theory", *Journal of Chemical Physics* **109**, 108 (1998)
6. G. E. Froudakis, **G. S. Fanourgakis**, S. C. Farantos and S. S. Xantheas, "Binding energies and structures of C^+Ar_n ($n = 1 - 5$), clusters from first principles", *Chemical Physics Letters* **294**, 109 (1998)
7. **G. S. Fanourgakis**, S. C. Farantos, Ch. Lüder, M. Velegrakis and S. S. Xantheas, "Photofragmentation spectra and potential energy surfaces of Sr^+Ar_2", *Physical Chemistry Chemical Physics* **1**, 977 (1999)
8. **G. S. Fanourgakis**, V. Pontikis, and G. Zérah, "Phase stability and intrinsic stacking faults in aluminum under pressure", *Physical Review B* **67**, 094102 (2003)
9. **G. S. Fanourgakis**, P. Parneix and Ph. Bréchignac, "Probing the liquid-gas like phase transition in the mixed Ar_xNe_{13-x} clusters?", *The European Physical Journal D*, **24**, 207 (2003)
10. **G. S. Fanourgakis**, Y. J. Shi, S. Consta, and R. H. Lipson, "A spectroscopic and computer simulation study of butanol vapors", *Journal of Chemical Physics* **119**, 6597 (2003)
11. **G. S. Fanourgakis**, E. Aprá and S. S. Xantheas, "High-level ab initio calculations for the four low-lying families of minima of $(H_2O)_{20}$: I. Estimates of MP2/CBS binding energies and comparison with empirical potentials", *Journal of Chemical Physics* **121**, 2655 (2004)
12. **G. S. Fanourgakis**, E. Aprá, W. A. de Jong, and S. S. Xantheas, "High-level ab initio calculations for the four low-lying families of minima of $(H_2O)_{20}$: II. Spectroscopic signatures of the dodecahedron, fused cubes, face-sharing pentagonal prisms, and edge-sharing pentagonal prisms hydrogen bonding networks", *Journal of Chemical Physics* **122**, 134304 (2005)
13. A. Lagutschenkov, **G. S. Fanourgakis**, G. Niedner-Schatteburg and S. S. Xantheas, "The spectroscopic signature of the "all-surface" to "internally solvated" structural transition in water clusters in the n=17-21 size regime", *Journal of Chemical Physics* **122**, 194310 (2005)
14. **G. S. Fanourgakis** and S. S. Xantheas, "The flexible, polarizable, Thole-type interaction potential for water (TTM2-F) revisited", *Journal Physical Chemistry A* **110**, 4100 (2006)
15. **G. S. Fanourgakis** and S. S. Xantheas, "The bend angle of water in ice Ih and liquid water: The significance of implementing the non-linear monomer dipole moment surface in classical interaction potentials", *Journal of Chemical Physics* **124**, 174504 (2006)
16. **G. S. Fanourgakis**, G. K. Schenter and S. S. Xantheas, "A quantitative account of quantum effects in liquid water", *Journal of Chemical Physics* **125**, 141102 (2006)
17. **G. S. Fanourgakis**, V. Tipparaju, J. Nieplocha and S. S. Xantheas, "An efficient parallelization scheme for molecular dynamics simulations with many-body, flexible, polarizable empirical potentials: Application to water", *Theoretical Chemistry Accounts* **117**, 73 (2007)
18. **G. S. Fanourgakis** and S. S. Xantheas, "Development of transferable interaction potentials for water. V. Extension of the flexible, polarizable, Thole-type model potential (TTM3-F, v. 3.0) to describe the vibrational spectra of water clusters and liquid water", *Journal of Chemical Physics* **128**, 074506 (2008)

19. S. Habershon, **G. S. Fanourgakis** and D. Manolopoulos, "Comparison of path integral molecular dynamics methods for the infrared absorption spectrum of liquid water", *Journal of Chemical Physics* **129**, 074501 (2008)
20. M. V. Kirov, **G. S. Fanourgakis** and S. S. Xantheas, "Identifying the most stable networks in polyhedral water clusters", *Chemical Physics Letters* **461**, 180 (2008)
21. M. L. Lipciuc, F. Wang, X. Yang, T. N. Kitsopoulos, **G. S. Fanourgakis** and S. S. Xantheas, "Cluster-controlled photofragmentation: The case of the Xe-Pyrrole cluster", *ChemPhysChem* **9**, 1838 (2008)
22. **G. S. Fanourgakis***, T. E. Markland and D. E. Manolopoulos, "A fast path integral method for polarizable force fields", *Journal of Chemical Physics* **131**, 094102 (2009)
23. M. Massaouti, **G. S. Fanourgakis** and M. Velegrakis, "Photodissociation spectroscopy and ab initio calculations for the $Sr^{+}N_2$ complex", *Chemical Physics Letters* **490**, 138 (2010)
24. J. Liu, W. H. Miller, **G. S. Fanourgakis**, S. S. Xantheas, S. Imoto and S. Saito, "Insights in quantum dynamical effects in the infrared spectroscopy of liquid water from a semiclassical study with an ab initio-based flexible and polarizable force field", *Journal of Chemical Physics* **135**, 244503 (2011)
25. **G. S. Fanourgakis***, J. S. Medina and R. Prosmiti. "Determining the Bulk Viscosity of Rigid Water Models", *Journal Physical Chemistry A* **116**, 2564 (2012)
26. D. Arismendi-Arrieta, J. S. Medina, **G. S. Fanourgakis**, R. Prosmiti and G. Delgado-Barrio. "Simulating liquid water for determining its structural and transport properties", *Applied Radiation and Isotopes* **83**, 115 (2014)
27. **G. S. Fanourgakis**, "An Extension of Wolf' s Method for the Treatment of Electrostatic Interactions: Application to Liquid Water and Aqueous Solutions", *Journal Physical Chemistry B* **119**, 1974 (2015)
28. M. Kanakidou,S. Myriokefalitakis, N. Daskalakis, G. Fanourgakis, A. Nenes, A. R. Baker, K. Tsigaridis, N. Mihalopoulos, "Past, Present, and Future Atmospheric Nitrogen Deposition", *Journal of the Atmospheric Sciences* **73**, 2039 (2016)
29. N. Daskalakis, K. Tsigaridis, S. Myriokefalitakis, **G. S. Fanourgakis**, M. Kanakidou, "Large gain in air quality compared to an alternative anthropogenic emissions scenario", *Atmospheric Chemistry and Physics* **16**, 9771-9784 (2016)
30. S. Myriokefalitakis, N. Daskalakis **G. S. Fanourgakis**, A. Voulgarakis, M. C. Krold, J. M. J. Aan de Brugh, M. Kanakidou, "Ozone and carbon monoxide budgets over the Eastern Mediterranean", *Science of the Total Environment* **563-564**, 40-52 (2016)
31. P. Hamm **G. S. Fanourgakis** and S. S. Xantheas, "A surprisingly simple correlation between the classical and quantum structural networks in liquid water", *Journal Chemical Physics* **147**, 064506 (2017)
32. D. P. Broom, C. J. Webb, **G. Fanourgakis**, G. E. Froudakis, P. N. Trikalitis, M. Hirscher, "Concepts for improving hydrogen storage in nanoporous materials". *International Journal of Hydrogen Energy* **44**, 7768 (2019)
33. **G. S. Fanourgakis**, Kanakidou, M. and Nenes, A. and Bauer, S. E. and Bergman, T. and Carslaw, K. S. and Grini, A. and Hamilton, D. S. and Johnson, J. S. and Karydis, V. A. and Kirkevåg, A. and Kodros, J. K. and Lohmann, U. and Luo, G. and Makkonen, R. and Matsui, H. and Neubauer, D. and Pierce, J. R. and Schmale, J. and Stier, P. and Tsigaridis, K. and van Noije, T. and Wang, H. and Watson-Parris, D. and Westervelt, D. M. and Yang, Y. and Yoshioka, M. and Daskalakis, N. and Decesari, S. and Gysel Beer, M. and Kalivitis, N. and Liu, X. and Mahowald, N. M. and Myriokefalitakis, S. and Schrödner, R. and Sfakianaki, M. and Tsimpidi, A. P. and Wu, M. and Yu, F. "Evaluation of global simulations of aerosol number and cloud condensation nuclei, and implications for cloud droplet formation", *Atmos. Chem. and Phys.* **19**, 8591 (2019)

34. **G. S. Fanourgakis**, K. Gkagkas, E Tylianakis, E. Klontzas, and G. Froudakis, "A Robust Machine Learning Algorithm for the Prediction of Methane Adsorption in Nanoporous Materials" *J. Phys. Chem. A* **123**, 6080 (2019)
35. **G. S. Fanourgakis**, K. Gkagkas, E Tylianakis and G. Froudakis, "A Universal Machine Learning Algorithm for Large Scale Screening of Materials", *J. Am. Chem. Soc.* **142**, 3814 (2020)
36. **G. S. Fanourgakis**, K. Gkagkas, E Tylianakis and G. Froudakis, "A Generic Machine Learning Algorithm for the Prediction of Gas Adsorption in Nanoporous Materials" *J. Phys. Chem. C*, **124**, 7117 (2020)
37. I. Tsamardinos, **G. S. Fanourgakis**, E. Greasidou, E. Klontzas, K. Gkagkas and G. E. Froudakis "An Automated Machine Learning Architecture for the Accelerated Prediction of Metal-Organic Frameworks Performance in Energy and Environmental Applications.", *Micropor. Mesopor. Mat.*, **300**, 110160 (2020)
38. **G. S. Fanourgakis**, K. Gkagkas, E. Tylianakis and G. E. Froudakis, "Fast Screening of Large Databases for Top Performing Nanomaterials using a Self-Consistent, Machine Learning based Approach" *J. Phys. Chem. C*, **124**, 19639 (2020)
39. **G. S. Fanourgakis**, K. Gkagkas and G. E. Froudakis, "Artificial MOFs with superior adsorption properties for extrapolation in Machine Learning." *J. Chem. Phys.* **156**, 054103 (2021)
40. L. Zhang, M. D. Allendorf, R. Balderas-Xicohténcatl, D. P. Broom, **G. S. Fanourgakis**, G. E. Froudakis, T. Gennett, K. E. Hurst, S. Ling, C. Milanese, P. A Parilla, D. Pontiroli, M. Ricco, S. Shulda, V. Stavila, T. A. Steriotis, C. J. Webb, M. Witman and M. Hirscher, "Fundamentals of hydrogen storage in nanoporous materials." *Prog. Energy* **4**, 042013 (2022)
41. J. Iskandarov, **G. S. Fanourgakis**, S. Ahmed, Waleed Alameri, G. E. Froudakis, G. N. Karanikolos "Data-driven prediction of in situ CO2 foam strength for enhanced oil recovery and carbon sequestration", *RSC Advances* in Press (2022)

Google Scholar citations: 2,537 **H-index: 25**

Participation in Scientific Conferences/Meetings

1. "Global simulations of Ice Nuclei Particles of Terrestrial and Marine Origin"
   Marios Chatziparaschos, Stelios Myriokefalitakis, George S. Fanourgakis, Dimitrios G. Amanatidis and Maria Kanakidou, EGU General Assembly 2019, Vienna, Austria 7-12 April 2019
2. " Organic aerosols and their impact on biogeochemical cycles and climate"
   Maria Kanakidou, Stelios Myriokefalitakis, Giorgos Fanourgakis, Marios Chatziparaschos, Kostas Tsigaridis, Athanassios Nenes, IGAC 2018 15th Science Conference, Takamatsu, Kagawa, Japan 25-29 September 2018
3. "Large-scale screening of Metal-Organic Frameworks (MOFs) using machine learning techniques"
   George S. Fanourgakis and George Froudakis, Energy Landscapes 2018 Kalamata, Greece 2-9 September 2018
4. "Evaluation and intercomparison of the aerosol number concentrations, CCNs and Cloud Droplets in global models"
   George S. Fanourgakis, Maria Kanakidou, Nikos Daskalakis, Stelios Myriokefalitakis, Athanassios Nenes, Risto Makkonen, Alf Grini, Alf Kirkeväg, Philip Stier, Duncan Watson-Parris, Nick Schutgens, Neubauer David, Lohmann Ulrike, Yang Yang, Hailong Wang, Ken Carslaw, Jeffrey Pierce, Jack Kodros, Peter Adams, Yunhaa Lee, Dan Westervelt, Douglas Stephen Hamilton, Hitoshi Matsui, Natalie M. Mahowald, Gan Luo, Fangqun Yu, Stefano Decesari, Cristina Facchini, Schmale Julia Yvonne, Urs Baltensperger, EGU General Assembly 2017, Vienna, Austria 22-29 April 2017

5. “Evaluation and intercomparison of the aerosol number concentrations and CCNs in global models” George S. Fanourgakis, Stelios Myriokefalitakis, Maria Kanakidou, Risto Makkonen, Alf Grini, Philip Stier, Duncan Watson-Parris, Nick Schutgens, Neubauer David, Lohmann Ulrike, Stefano Decesari, Cristina Facchini, Schmale Julia Yvonne, Urs Baltensperger, BACCHUS Annual Meeting 2017, ETH Zürich, Switcherland 10-12 January 2017
6. “The contribution of bioaerosols to the organic carbon of the atmosphere” S. Myriokefelitakis, G. S. Fanourgakis, M. Kanakidou, 13th International Conference on Meteorology, Climatology and Armospheric Physics (COMECAP2016) Aristotle Univ. of Thessaloniki, Greece 19-21 September 2016
7. “Study of the CCN formation as a function of aerosol components” G. S. Fanourgakis, S. Myriokefalitakis, M. Kanakidou, “The contribution of bioaerosols to the organic carbon of the atmosphere” S. Myriokefelitakis, G. S. Fanourgakis, M. Kanakidou, EGU General Assembly 2016, Vienna, Austria 17-22 April 2016
8. ”Improving the efficiency and accuracy of chemical kinetic solvers used in climate simulations” D. Taraborrelli, G. S. Fanourgakis, A. Pozzer, B. Steil and J. Lelieveld, Energy, Water and Climate Change (EWACC) 2012 Conference, Nicosia, Cyprus 10-12 December 2012
9. ”Calculations of the viscosities of liquid water by molecular simulations with polarizable interaction potentials” G.S. Fanourgakis, J.S. Medina, R. Prosmiti, P.Villarreal, G. Delgado-Barrio, World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostela, Spain 17-22 July 2011
10. ”A fast path integral method for polarizable force fields. Application to liquid water and Ice” G. S. Fanourgakis, T. E. Markland and D. E. Manolopoulos, International Meeting on Atomic and Molecular Physics and Chemictry, Madrid, Spain, 29-June-2 July 2010
11. ”Ab initio studies of the major families of minima for $(H_2O)_{20}$: Identifying the most stable networks in polyhedral water clusters” G. S. Fanourgakis, M. V. Kirov, S. S. Xantheas, S3C 2009: Conference on Size Selected Clusters, Brand, Austria, 8-13 March 2009
12. ”Low-energy networks of water cages and extended hydrate host lattices” M. V. Kirov, S. Yoo, G. S. Fanourgakis and S. S. Xantheas, S3C 2009:S3C 2009: Conference on Size Selected Clusters, Brand, Austria, 8-13 March 2009
13. ”An ab-initio based transferable interaction potential for water”, G. S. Fanourgakis and S. S. Xantheas, ACS National meeting, Salt Lake City, Utah, USA March 2009
14. ”Development of a transferable interaction potential for water from first principles: Extension of the TTM potential (version 3.0) to describe the vibrational spectra of water clusters and the liquid”, G. S. Fanourgakis and S. S. Xantheas, ACS National meeting, Boston, MA, USA August 2007
15. ”A quantitative account of quantum effects in liquid water”, G. S. Fanourgakis, G. K. Schenter and S. S. Xantheas, New Zealand Institute of Chemistry NZIC 2006, New Zealand December 2006
16. ”The bend angle of water in ice Ih: The significance of implementing the non-linear monomer Dipole Moment Surface in classical interaction potentials”, G. S. Fanourgakis and S. S. Xantheas, 11th International Conference on the Physics and Chemistry of Ice, Bremerhaven, Germany, 23-28 July 2006
17. ”High level ab initio calculations for the four low lying families of minima of $(H_2O)_{20}$: Spectroscopic signatures and estimates of MP2/CBS binding energies” G. S. Fanourgakis, E. Apra, W. A. de Jong, S. S. Xantheas, Pacifichem 2005, Honolulu, HI, USA 15-20 December 2005
18. ”Quantum dynamical simulations of liquid water with the TTM2-F interaction potential”, G. S Fanourgakis, G. K. Schenter and S. S. Xantheas, Pacifichem 2005, Honolulu, HI, USA 15-20 December 2005

19. "Strong vs weak nearest-neighbor hydrogen bonds in water clathrates: Interplay between relative stability and IR spectral features", M. V. Kirov, G. S. Fanourgakis and S. S. Xantheas, Symposium: Electric (hyper)polarizability: From atoms and molecules to the nonlinear optics of materials, Corinth, Greece 21-26 October 2005
20. "High-Level ab initio calculations for the four low-lying families of minima of $(H_2O)_{20}$: II. Spectroscopic signatures of the dodecahedron, fused cubes, face-sharing, and edge-sharing pentagonal prisms hydrogen bonding networks.", G. S. Fanourgakis, E. Apra and S. S. Xantheas, EMSI International Workshop on Ions and Molecules at Aqueous Interfaces, Prague, Czech Republic, 27 June 2005
21. "Structural, spectral and excited state features of water hydrogen bonding networks: Results of ab-initio calculations and interaction potentials", G. S. Fanourgakis, A. Lagutschenkov, K. Kowalski, G. Niedner-Schatteburg and S. S. Xantheas, 229th ACS National Meeting, San Diego, CA, USA, 13-17 March 2005
22. "Quantum dynamical simulations of liquid water with the TTM2-F interaction potential", G. S. Fanourgakis, G. K. Schenter and S. S. Xantheas, 229th ACS National Meetings, San Diego, CA, USA, 13-17 March 2005
23. "Structural, and spectral features of size selected water clusters in the $n = 7 - 21$ regime: Results from electronic structure calculations and empirical potentials", G. S. Fanourgakis, A. Lagutschenkov, G. Niedner-Schateburg, and S. S. Xantheas, S3C 2005: Conference on Size Selected Clusters, Brand, Austria 28 February - 3 March 2005
24. "Spectroscopic signatures of the four low-lying families of minima of $(H_2O)_{20}$ water clusters", G. S. Fanourgakis, E. Apra, W. A. de Jong, and S. S. Xantheas, Gordon Research Conference, "Molecular and Ionic Clusters", Centre Paul Langevin, Aussois, France 4-11 September 2004
25. "Investigation of the accuracy of several empirical potentials for the description of clusters and crystalline Ice", G. S. Fanourgakis, E. Apra, S. S. Xantheas, Telluride Summer Workshop: "Ice, Icy Surfaces and Ice Particles", Telluride, Colorado, USA 25-31 July 2004
26. "The relative stability of the major families of local minima of $(H_2O)_{20}$: Results of high-level ab-initio calculations and comparison with empirical potentials", G. S. Fanourgakis and S. S. Xantheas, Theory and Applications in Computational Chemistry (TACC), Korea 2004
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8. Journal of Physics: Condensed Matter
9. Journal of Physical Chemistry
10. Chemical Physics Letters
11. Chemical Engineering Science
12. Computational Materials Science
13. Materials Today Communication
14. Microporous and Mesoporous Materials
15. Journal of Environmental Chemical Engineering
16. Nanomaterials
17. Advanced Theory and Simulations
18. Reviewer of reserach proposals for the National Science Foundation (NSF) of the US.