Dr. Styliani Consta

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EDUCATION

Ph.D. Department of Chemistry, Chemical Physics Theory Group, University of Toronto. *Dissertation Title* : "Ion transfer reactions in clusters". *Adviser* : Professor Raymond Kapral

M.Sc. Department of Chemistry, Queen's University, Kingston, Ontario. *Dissertation Title* : "An ab initio study of the hyperfine frequency shift of atomic Hydrogen in Helium buffer gas". *Adviser* : Professor Vedene Smith

Research Assistant at the National Hellenic Research Foundation (NHRF), Athens, Greece

Bachelor degree in Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Greece.

Languages: English, Greek, French

EMPLOYMENT HISTORY

Professor, Department of Chemistry, The University of Western Ontario

Associate Professor, Department of Chemistry, The University of Western Ontario.

Assistant Professor, Department of Chemistry, The University of Western Ontario.

Marie Curie Fellow. in Computational Physics, F.O.M. Institute for Atomic and Molecular Physics (AMOLF), Amsterdam, The Netherlands. Adviser: Prof. Daan Frenkel
https://cordis.europa.eu/project/id/FMBI972312 Project title: "Effects of solvation of aerosol sodium chloride crystals on atmospheric reactions"

Teaching Assistant at the University of Toronto (Ph.D. Candidate).

Teaching Assistant at Queen's University (M.Sc. Candidate).

Areas of Academic Responsibility, Dept. of Chemistry, UWO (1999-current):

Teaching: 40 %, Research: 40 %, Service: 20 %

HONORS AND AWARDS

2022 Fulbright Canada Research Chair in Climate Change, Air Quality, and Atmospheric Chemistry, University of California, Irvine, 2022-2023

2021 Department of Chemistry (UWO) Research Excellence Award

2014/16 Marie Curie International Incoming Fellowship (IIF), Department of Chemistry University of Cambridge, UK (Europe)

2014/16 Elected visiting Fellow, Lucy Cavendish College, University of Cambridge, UK

2003 NSERC Accelerator Grant for Exceptional New Opportunities

2001/06 Premier's Research Excellence Award (Canada)

1997/99 Marie Curie Research Training Grant (The Netherlands)

1994/96 University of Toronto Open Fellowship (Canada)

1993/94 Ontario Graduate Scholarship (Canada)

1991/92 Queen's University Dean's Award (Canada)

1990/91 Queen's University Graduate Award (Canada)
1989/90 National Hellenic Research Foundation Scholarship (Greece)

Visiting Scientist

March 2022/ August 2022 Fulbright Canada Research Chair in Climate Change, Air Quality, and Atmospheric Chemistry, University of California, Irvine.
March 2019/ June 2019 Visiting Scientist, John A. Paulson School of Engineering and Applied Sciences, Harvard, US.
May 2017/ August 17 Visiting Scientist, Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
July 2014/ August 16 Visiting Fellow at the Lucy Cavendish College, University of Cambridge, UK (applied for and elected by the Governing Body of the College).
July 2014/ August 16 Marie Curie Fellow at the Department of Chemistry, University of Cambridge, UK (Computational/Theoretical Group).
January 2006/ April 06 Visiting Scientist at the Department of Chemistry, Physical and Theoretical Chemistry, Technical University of Munich, Munich, Germany (Hosts: Prof. Dr. W. Domcke, Dr. M. Thoss)

RESEARCH

Research interests

Computational physical chemistry and biochemistry, atmospheric aerosols, chemistry in confining environments such as clusters and droplets, ion-solvent interactions, liquid-vapour interfaces, biological macromolecules, protein complexes, electric double layer, modelling ionization methods in analytical chemistry.

Methods: statistical mechanics, molecular simulations, mathematical modelling, molecular dynamics, ab initio molecular dynamics, look-ahead Monte Carlo methods, rare event dynamics, free energy calculations, multi-scale modelling, non-linear Poisson-Boltzmann equation.

Publications

The corresponding author carries an asterisk, graduate students are indicated by (G) and undergraduates by (U). All the publications have been funded by NSERC. In the most of the publications there is long supporting information (SI) that accompanies the main article and has significant information such as studies of different systems that support the material of the main article, and analytical theory.

1. **S. Consta*** "Modelling the chemistry in droplets across size scales" Invited perspective article in Physical Chemistry Chemical Physics (in preparation).
2. Marko Voronych **(U)** and **S. Consta*** "Cone angle and dynamics in "star"-like shaped droplets" (in preparation).
3. Han Nguyen **(G)** and **S. Consta*** "Ion-pairing and diffusion in charged droplets at room temperature and supercooling" (in preparation) (2025).
4. Jihong Shi **(PDF)**, Han Nguyen **(G)**, Mateo Pescador Arboleda **(U)**, **S. Consta*** (first and last authors have equal contribution) "From sphere to cones: Structural instabilities and acidity at conical regions in trivalent metal ion nano-clusters", submitted to the Journal of the American Chemical Society (ja-2025-068798) (2025). 10.26434/chemrxiv-2025-9b03l *Revisions were submitted, Under review*
5. **S. Consta***, Han Nguyen **(G)** "Molecular simulation methods of evaporating electrosprayed droplets", International Journal of Mass Spectrometry, **508**, 117369 (2025).
6. **S. Consta***, L. M. Wingen, Y. Qin, V. Perraud, & B. J. Finlayson-Pitts, "Modeling the ionization mechanism of amorphous solid particles without an external energy source coupled to mass spectrometry", Physical Chemistry

Chemical Physics, **26**, 28220-28233 (2024).

7. Victor Kwan **(G)**, **S. Consta***, Shahrazad M. A. Malek, "The variation of surface propensity of halides with droplet size and temperature. The planar interface limit" The Journal of Physical Chemistry B, 128(1), 193-207 (2023).
8. Victor Kwan **(G)**, Pranav Ballaney **(U)**, Titiksha **(U)**, **S. Consta*** "Limitations of atomistic molecular dynamics to reveal ejection of proteins from charged nanodroplets", The Journal of Physical Chemistry B **127** (20): 4829–4842 (2023).
9. **S. Consta*** "Atomistic modeling of jet formation in charged droplets ", Journal of Physical Chemistry B **126** (41): 8350–8357 (2022).
10. V. Kwan **(G)**, **S. Consta*** "Conical shape fluctuations determine the ejected cluster-size distribution and emission rate of ion-evaporation from multiple-charged droplets", Journal of Physics Chemistry A **126** (20): 3229–3238 (2022).
11. V. Kwan **(G)**, S. R. Maiti **(U)**, Ivan Saika-Voivod, **S. Consta*** "Salt enrichment and dynamics in the interface of a supercooled aqueous droplet", Journal of the American Chemical Society **144** (25): 11148-11158 (2022).
12. S. M. A. Malek, V. Kwan **(G)**, Ivan Saika-Voivod, **S. Consta***, "Low density interior in super-cooled aqueous nanodroplets expels ions to the subsurface", Journal of the American Chemical Society **143** (33): 13113-13123 (2021).
13. V. Kwan **(G)**, Ryan O'Dwyer **(U)**, David Laur **(U)**, Jiahua Tan **(U)**, **S. Consta*** "The relation between ejection mechanism and ion abundance in the electic double layer of droplets", Journal of Physical Chemistry A **125**: 2954–2966 (2021).
14. V. Kwan **(G)**, **S. Consta***, "Molecular characterization of the surface excess charge layer in droplets" Journal of the American Society for Mass Spectrometry **32**: 33–45 (2020).
15. V. Kwan **(G)**, **S. Consta*** "Bridging electrostatic properties between nanoscopic and microscopic highly charged droplets" Chemical Physics Letters, **746**: 137238 (2020).
16. V. Kwan **(G)**, A. Malevanets, **S. Consta*** "Where do the ions reside in a highly charged droplet?" Journal of Physical Chemistry A **123**(43): 9298–9310 (2019).
17. M. In Oh **(G)**, **S. Consta*** "General solvation motifs of a charged linear macroion in an aqueous droplet" Molecular Physics **117**: 2889-2899 (2019).
18. M. Sharawy **(G)**, **S. Consta*** "Effect of the chemical environment of the DNA guanine quadruplex on the free energy of binding of Na and K ions" Journal of Chemical Physics **149**.22: 225102 (2018).
19. **S. Consta***, M. In Oh **(G)**, V. Kwan **(G)**, A. Malevanets, "Strengths and weaknesses of molecular simulations of electrosprayed droplets", Critical Insight in the Journal of the American Society for Mass Spectrometry, **29**(12): 2287–2296 (2018).
20. A. Malevanets, M. In Oh **(G)**, M. Sharawy **(G)**, **S. Consta*** "Landau-Ginzburg theory for the "star"-shaped droplets" Molecular Physics, **116.21-22**: 2892-2900 (2018).
21. **S. Consta***, M. In Oh **(G)**, M. Sharawy **(G)**, A. Malevanets "Macroion-solvent interactions in charged droplets", Invited **feature and cover article** in the Journal of Physical Chemistry A, **122**(24): 5239–5250 (2018).
22. M. In Oh **(G)**, M. Paliy, **S. Consta*** "Star" morphologies of charged nanodrops comprised of conformational isomers" Journal of Chemical Physics, **148.2**: 024307 (2018).
23. **S. Consta***, A. Malevanets, M. In Oh **(G)**, M. Sharawy **(G)**, "Role of a reaction coordinate in free energy calculations" Molecular Physics **44**:1033–1043 (2018).
24. M. In Oh **(G)**, A. Malevanets, M. Paliy, D. Frenkel*, **S. Consta*** "When droplets become stars: charged dielectric droplets beyond the Rayleigh limit" Soft Matter **13**: 8781–8795 (2017).
25. M. In Oh **(G)**, **S. Consta*** "What Factors Determine the Stability of a Weak Protein-Protein Interaction in a Charged Aqueous Droplet?" Physical Chemistry Chemical Physics **19**: 31965–31981 (2017).
26. **S. Consta***, M. Sharawy **(G)**, M. In Oh **(G)**, A. Malevanets "Advances in modeling the stability of non-covalent complexes in charged droplets with applications in ESI-MS experiments" Invited Perspective article in Ana-

lytical Chemistry **89**: 8192–8202 (2017).
27. Myong In Oh **(G)** and **S. Consta*** "Charging and release mechanisms of flexible macromolecules in droplets" Journal of the American Society for Mass Spectrometry **28**: 2262–2279 (2017).
28. Myong In Oh **(G)** and **S. Consta*** "Stability of a transient protein complex in a charged aqueous droplet with variable pH", Journal of Physical Chemistry Letters, **8**: 80-85 (2017).
29. M. Sharawy **(G)** and **S. Consta*** "Characterization of "star" droplet morphologies induced by charged macromolecules" The Journal of Physical Chemistry A, **120**: 8871–8880 (2016).
30. **S. Consta***, Myong In Oh **(G)**, A. Malevanets "New mechanisms of macroion-induced disintegration of charged droplets" Invited article in Chemical Physics Letters-Frontiers, **663**: 1–12 (2016).
31. M. Sharawy **(G)**and **S. Consta*** "How do non-Covalent Complexes Dissociate in Droplets? A case study of the Desolvation of dsDNA from a charged aqueous nanodrop" *Physical Chemistry Chemical Physics* **17**: 25550–25562 (2015).
32. Sepideh Soltani **(G)**, Myong In Oh **(G)**, **S. Consta*** "Effect of solvent on the charging mechanisms of poly (ethylene glycol) in droplets" Journal of Chemical Physics **142**: 114307 (2015).
33. **S. Consta***, A. Malevanets "Disintegration mechanisms of charged Nanodroplets: Novel systems for applying methods of activated processes" Molecular Simulation **41**: 73-85 (2015); Invited review article in special Issue on recent advances in the molecular simulation of chemical reactions.
34. **S. Consta***, Myong In Oh **(G)**, Sepideh Soltani **(G)** "Advances in the theoretical and molecular simulation studies of the ion chemistry in droplets" International Journal of Mass Spectrometry **377**: 557–567 (2015). Invited article in the Special Issue of the International Journal of Mass Spectrometry Edited By Jean Futrell and Michael Bowers "MS 1960 to Now". This was the only theoretical article that was invited for the issue.
35. F. Sheriff **(U)** and **S. Consta*** "Charge-Induced Instabilities of Droplets Containing Macromolecular Complexes", Canadian Journal of Chemistry–Revue Canadienne de Chimie, **93**: 1-8 (invited article) (2014).
36. M. Sharawy **(G)** and **S. Consta*** "Effect of counterions on the charging mechanisms of a macromolecule in aqueous nanodrops", Journal of Chemical Physics **141**: 104321 (2014).
37. M. Paliy, **S. Consta*** and J. Yang "Interactions between carbon nanoparticles in a droplet of organic solvent" Journal of Physical Chemistry C **118**: 16074-16086 (2014).
38. A. Buin, H. Wang **(G)**, **S. Consta***, Y. Huang* "A Study of Conformational Equilibrium of 1,1,2-Trichloroethane in FAU-type Zeolites" Microporous and Mesoporous Materials **183**: 207-217 (2014).
39. A. Malevanets and **S. Consta*** "Variation of droplet acidity during evaporation" Journal of Chemical Physics **138**: 184312 (2013).
40. **S. Consta*** and A. Malevanets "Classification of charged induced instabilities in droplets with macromolecules" Journal of Chemical Physics **138**: 044314 (2013).
41. **S. Consta*** and A. Malevanets "Manifestations of charge induced instability in droplets effected by charged macromolecules" Physical Review Letters **109**(14) :148301 (2012).
42. Doaa M. Ragab **(G)**, S. Rohani* and **S. Consta** "Controlled Release of 5-Fluorouracil and Progesterone from Magnetic Nano-Aggregates", International Journal of Nanomedicine **7**: 3167–3189 (2012).
43. Jun Kyung Chung and **S. Consta*** " "Release mechanisms of poly(ethylene glycol) macroion from aqueous charged nanodroplets" Journal of Physical Chemistry B **116** (19) : 5777-5785 (2012).
44. A. Buin, J. Ma **(G)**, Y. Huang and **S. Consta***, Z. Hui " Conformational Changes of trans-1,2-Dichlorocyclohexane Adsorbed in Zeolites Studied by FT-Raman Spectroscopy and Molecular QM/MM Simulations", Journal of Physical Chemistry C **116** (15) :8608-8618 (2012).
45. M. Paliy, O.M. Braun*, **S. Consta*** "Friction in a thin water layer: dissociative versus non-dissociative friction" Journal of Physical Chemistry C **116**(16): 8932-8942 (2012).
46. A. Buin and **S. Consta*** and Tsun-Kong Sham "Mechanisms of phase transformations of TiO_2 nanotubes and nanorods" Journal of Physical Chemistry C **115**(45): 22257-22264 (2011).
47. **S. Consta*** and Jun Kyung Chung "Charge-Induced Conformational Changes of PEG-$(Na^+)_n$ in vacuum and

aqueous nanodroplets" Journal of Physical Chemistry B **115**(35): 10447–10455 (2011).
48. **S. Consta*** "Manifestation of Rayleigh instability in droplets containing multiply charged macroions" Journal of Physical Chemistry B **114**(16): 5263–5268 (2010).
49. Y. Liu, **S. Consta*** and W. A. Goddard III*, "Nanoimmiscibility: Selective absorption of liquid methanol-water mixtures in carbon nanotubes" Journal of Nanoscience and Nanotechnology **10**(6) : 3834–3843 (2010).
50. Y. Liu, **S. Consta***, Y.J. Shi **(G)**, R.H. Lipson, W. A. Goddard III*, "Prediction of the size distributions of Methanol-Ethanol clusters detected in VUV Laser/Time-of- Flight Mass Spectrometry" Journal of Physical Chemistry A **113** (25): 6865–6875 (2009)
51. Liu Y., **S. Consta***, Ogeer F. **(G)**, et al. "Geometries and energetics of methanol-ethanol clusters: a VUV laser/time-of-flight mass spectrometry and density functional theory study" Canadian Journal of Chemistry-Revue Canadienne de Chimie **85** 10 :843–852 (2007).
52. **S. Consta*** "Detecting reaction pathways and computing reaction rates in condensed phase" **Invited refereed paper**, Theoretical Chemistry Accounts **116** (1-3): 373–382 (2006).
53. K. Ichiki, **S. Consta***. "Disintegration mechanisms of charged aqueous nanodroplets studied by simulations and analytical models." Journal of Physical Chemistry B **110**(39): 19168–19175 (2006).
54. M. Paliy, O. M. Braun*, **S. Consta***. "The friction properties of an ultrathin confined water film." Tribology Letters **23** (1): 7–14 (2006).
55. Y. Liu and **S. Consta*** "Dynamic breaking and restoring of finite water chains inside carbon nanotubes" Computing Letters **1**, 192–197 (2006) (Invited refereed paper).
56. O. M. Braun*, M. Paliy, **S. Consta*** "Ordering of a thin lubricant film due to sliding", Physical Review Letters **92**(25): 256103 (2004).
57. **S. Consta***, K. Mainer and W. Novak "Mechanisms of fragmentation processes of aqueous clusters charged with ions", Journal of Chemical Physics **119**: 10125 (2003).
58. G.S. Fanourgakis, Y.J. Shi **(G)**, **S. Consta***, R. H. Lipson* "A spectroscopic and computer simulation study of butanol vapours", Journal of Chemical Physics **119**(13):6597 (2003).
59. **S. Consta***. "Fragmentation reactions of charged aqueous clusters." J. Mol. Struc.-THEOCHEM **591**:131 (2002).
60. Y.J Shi **(G)**, **S. Consta***, A. K. Das, B. Mallik, **D. Lacey (U)** and R. H. Lipson*. "A 118 nm Vacuum Ultraviolet/Time of Flight Mass Spectroscopic Study of Methanol and Ethanol Clusters in the Vapour Phase." Journal of Chemical Physics **116**: 6990–6999 (2002).
61. R. Kapral* and **S. Consta** "Classical and Quantum Chemical Rate Constants for Reactions in Condensed Phases" CERAPIE: 253–269 (2002); **Invited Paper**. CERAPIE is a European Journal of pedagogical nature.
62. **S. Consta (G)** and R. Kapral*. "Ionization reactions of ion complexes in mesoscopic water clusters." Journal of Chemical Physics **111**:10183-10191 (1999).
63. **S. Consta**, N.B. Wilding, D. Frenkel, and Z. Alexandrowitz*. "Recoil growth: an efficient simulation method for multi-polymer systems." Journal of Chemical Physics, **110**: 3220–3228 (1999).
64. **S. Consta**, T.J.H. Vlugt **(G)**, J.W. Hoeth **(G)**, B. Smit and D. Frenkel*. "Recoil Growth Algorithm for Chain Molecules with Continuous Interactions." Journal of Molecular Physics, **97**: 1243–1254 (1999).
65. R. Kapral*, **S. Consta (G)**, and D. Laria. "Proton reactions in clusters." Canadian Journal of Chemistry-Revue Canadienne de Chimie, **75**: 1–8 (1997). (Feature article).
66. **S. Consta** and R. Kapral*. "Dynamics of proton transfer in mesoscopic clusters." Journal of Chemical Physics, **104**(12): 4581–4590 (1996).
67. **S. Consta (G)** and R. Kapral*. "Proton transfer in mesoscopic molecular clusters." Journal of Chemical Physics, **101**:10908–10914 (1994).
68. Petsalakis I.D.*, Theodorakopoulos G.*, **S. Consta** "Theoretical calculations on the electronic states of XeH" Molecular Physics, **75**(4): 805–810 (1992).

Conference Proceedings

- R. Kapral*, **S. Consta (G)**, and L. McWhirter **(G)**. "Chemical rate laws and rate constants." In *Classical and Quantum Dynamics in Condensed Phase Simulations*. Bruce J. Berne, Giovanni Ciccotti, and David F. Coker, editors, World Scientific, 583–616 (1998). (Refereed proceedings of the International School of Physics "Computer Simulation of Rare Events and the Dynamics of Classical and Quantum Condensed-Phase Systems.")

Conference Proceedings (non-referred)

Abstracts have been reviewed.

1. S. Consta*, J. Shi. "Rayleigh charge-induced instability in sub-nanometer aqueous clusters charged by a trivalent metal cation and multiple hydronium ions", Proceedings of the American Society for Mass Spectrometry Conference, Baltimore, Maryland, 2025.
2. S. Consta*, L. M. Wingen, Y. Qin, V. Perraud, B. J. Finlayson-Pitts*. "Protonation of analytes in ESI and matrix assisted ionization in vacuum modeled from the micro-scale to nano-scale", Proceedings of the American Society for Mass Spectrometry Conference, Anaheim, California, 2024.
3. L. M. Wingen*, Y. Qin, V. Perraud, S. Consta, E. Wingen, C. Begay, B. J. Finlayson-Pitts*. "Use of matrix assisted ionization in vacuum - Mass spectrometry to characterize the surface layers of organic particles", Proceedings of the American Society for Mass Spectrometry Conference, Anaheim, California, 2024.
4. S. Consta*, Y. Qin, L. Wingen, B. J. Finlayson-Pitts*. "Charging of analytes in droplets and solid particle-based ionization methods. Linking the chemistry between microscopic and nanoscopic-sized systems". Proceedings of the American Society for Mass Spectrometry Conference, Houston, Texas, 2023.

Other Scholarly and Professional Activities

Invited Talks at Conferences, Universities and Industries

1. S. Consta. "Supercooling of droplets and formation of amorphous ice", The McGill Molecular Science Mini-Meeting, Montreal, July 16-18, 2025. **International Meeting**
2. S. Consta. "Multiscale modeling of electrostatic phenomena and chemical reactivity in nanoscale to microscale droplets", Aqueous Systems: The Frontier and Beyond. Kalamata, Greece, June 15-21, 2025. (https://voices.uchicago.edu/sys/) **International Conference**
3. S. Consta. "Linking electrostatic properties between nanoscopic and microscopic droplets generated by electro-spraying", American Chemical Society (ACS), San Diego, March 23-27, 2025. **International Conference**
4. S. Consta. "Insight into Matrix Assisted Ionization in Vacuum - Mass Spectrometry by Molecular Modelling", 22th Toronto Post-ASMS Mass Spectrometry Symposium Organized by Canadian Forum for Analytical and Bioanalytical Sciences, Toronto, 2024.
5. S. Consta. "Ion-Water interactions in supercooled droplets", Gordon Research Conference "Water and Aqueous Solutions", July 21-24, 2024, Holderness, NH (Presentation date: July 22, 2024).
6. S. Consta. "Charging mechanism of macromolecules in droplet-based ionization methods revealed by multi-scale modelling", Department of Chemistry and Biochemistry, Concordia University, Montreal, March 22, 2024.
7. S. Consta. Sandia National Laboratories, Albuquerque, September 2023 (on-line).
8. S. Consta. 21th Toronto Post-ASMS Mass Spectrometry Symposium Organized by Canadian Forum for Analytical and Bioanalytical Sciences, Toronto, October 16, 2023.
9. S. Consta. "Charging of analytes in droplet and solid particle-based ionization methods. Linking the chemistry between microscopic and nanoscopic systems. American Society for Mass Spectrometry (ASMS), Houston, June 7,2023 (oral presentation, in-person); the conference has several thousands of participants and only 10% of the participants are given an oral presentation.
10. S. Consta. "Modeling of electrostatic and chemical properties of nanoscopic and microscopic aerosol droplets", Department of Chemistry, University of California, Irvine, March 14, 2023.
11. S. Consta. "Droplets at the Rayleigh limit: what we can learn from atomistic modelling", Atmospheric Aerosol

Research, Karlsruhe Institute of Technology, Germany, January 23, 2023 (on-line).
12. S. Consta. "Chemistry in small volumes: The story of a (macro)ion in a droplet", Dept. of Chemistry, UWO, January 11, 2023.
13. S. Consta. "Ions in Solution" Telluride, US (2023, invited, I could not attend).
14. S. Consta. "Chemistry in small volumes: From atmospheric aerosols to biological cells", Soochow University-Western University Center for Synchrotron Radiation Research (SWC) Annual workshop, November 23-24, 2022 (on-line).
15. S. Consta. Departmental Seminar in the Robert Frederick Smith School of Chemical and Biomolecular Engineering, Cornell University, October 3, 2022 (https://www.cheme.cornell.edu/events/cbe-seminar-styliani-consta)
16. S. Consta. **Plenary presentation**, Foundations of Molecular Modeling and Simulation (FOMMS) Conference, July 17-21, 2022, Delavan, WI, US. FOMMS is one of the **top simulation international conference**. FOMMS conferences typically have 120 to 180 international participants, in an interdisciplinary mix that includes chemical engineers, chemists, physicists, and materials and data scientists from both academia (including students and postdocs), government laboratories, and industry.
17. S. Consta. Seminar in the Department of Physics, University of Maryland, Baltimore County, November 10, 2021.
18. S. Consta. Seminar in the Department of Biochemistry, The University of Western Ontario, Title "Providing insight into the interactions of solvated simple and macro-ions using computer modelling", March 26, 2021.
19. S. Consta. Invited speaker in the Pacifichem, 2020 (transferred in December 2021). Title "Bridging electrostatic and surface properties between nanoscopic and microscopic charged droplets", Symposium: Structure and function of complex molecular clusters – challenges in theory and experiment.
20. S. Consta. Invited speaker in the Biophysical Society, Canada, 2020 (cancelled); The conference took place virtually in May 25-28, 2021. My invited seminar was on May 28, 2021.
21. S. Consta. Invited speaker in the 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, August 16-21, 2020, Vancouver, Canada. **International Conference** (cancelled). The conference took place July 3-8, 2022 and I delivered my presentation in-person.
22. S. Consta. 29th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Kelowna, British Columbia from August 10-14, 2020. **National Conference** (cancelled). The conference took place in July 2022. However, I could not attend because of difficulties to reach the conference place in time due to flight cancellations.
23. S. Consta. "Ions in Solution" Telluride, US (cancelled)
24. S. Consta. International Conference on Polymers and Advanced Materials POLYMAT-2019, Huatulco, Mexico, October 20-25, 2019. **International Conference** (declined)
25. S. Consta. "Ionic strength in systems that violate electric neutrality", American Chemical Society (ACS), San Diego, August 25-29, 2019. **International Conference**
26. S. Consta."Modeling protein complexes in solution" Invited Seminar, Department of Chemistry, January 10, 2019 University of Western Ontario.
27. S. Consta. Invited Seminar, Department of Applied Mathematics, University of Western Ontario, November 28, 2018.
28. S. Consta. "Extension of the Rayleigh theory for charged droplets - What Rayleigh could not have predicted" Invited Seminar, Department of Physics and Astronomy, University of Western Ontario, December 13, 2018.
29. S. Consta. "Toward an understanding of the protein-protein interactions" in "Energy Landscapes" meeting, Sept. 2-9, 2018, Kalamata, Greece. **International Conference**
30. S. Consta. "Investigating mechanisms of protein interactions", Tenth Liblice conference on the statistical mechanics of liquids", June 17-22, 2018, Srni, Czech Republic. **International Conference**
31. S. Consta. "Computational evidence of charging mechanisms of macromolecules in ESI droplets" and "Role of ions in protonation/deprotonation reactions with macroions" Oral presentations in the workshop of "The Black Box of Metal Ions and Counterions in Electrospray Ionization: Experimental and Computational Perspectives on the Charging Conditions in Droplets. American Society for Mass Spectrometry, San Diego, US June 5-June 8, 2018. **International Conference**
32. S. Consta. "Investigating the stability of interfaces in non-covalent protein complexes in solution", in the session of "Assessing Complex Free Energy Surfaces from Molecular Simulations from Electronic Structure to Mesoscopic Processes", Canadian Society for Chemistry Conference, Edmonton, May 27-June 1st, 2018. **International Conference**
33. S. Consta. "Star-shaped droplets: simulations and theoretical analysis of their origin and shape", Focus Program

on Nanoscale Systems and Coupled Phenomena: Mathematical Analysis, Modeling, and Applications, Interdisciplinary Seminars and Panel Discussions, Fields Institute, University of Toronto, Toronto, May 14-18, 2018. **National Conference**

34. S. Consta. "What are the factors that determine the stability of protein complexes in droplets?" **Hot topic presentation**, Sanibel Conference, Jan. 25-29, 2018, St. Petersburg, FL, US. **International Conference**
35. S. Consta. Invited Discussion Leader, in the Gordon Conference on "Chemistry and Physics of Liquids", August 6-11, 2017 at the Holderness School, Holderness, New Hampshire. **International Conference**
36. S. Consta. "A Computational Journey from Liquid Droplets Charged with Single Ions to Assemblies of Proteins" Group meeting presentation, CFEL (Center for Free Electron Laser), Max Planck Institute of the Structure and Dynamics of Matter, Hamburg, Germany, July 4, 2017.
37. S. Consta. Organize a session in 100th anniversary of CSC2017, Toronto, May 28-June 1st, 2017. The session was in the morning of May 29, 2017. **International Conference**
38. S. Consta. "Stability of protein complexes in droplets", 2017 Gordon Research Conference on Gaseous Ions: Structures, Energetics and Reactions, Ventura, CA, February 12-17, 2017. **International Conference**
39. S. Consta. "The desolvation mechanisms of macromolecules and of their complexes from charged droplets" Department of Chemistry, Wayne University, Detroit, US, February 22, 2017.
40. S. Consta. "Droplet Chemistry. The distinct droplet morphologies due to macroions", Department of Chemistry, McMaster University, November, 2016.
41. S. Consta. "Effect of droplet acidity in chemical reactivity and charge state of proteins", Department of Chemistry, University of Athens, Greece, November, 2016.
42. S. Consta. "When droplets become stars: charged droplets beyond Rayleigh instability", European Molecular Liquids Group (EMLG) and the Japanese Molecular Liquids Group (JMLG), September, 2016, Chania, Greece. **Invited Presentation, International Conference**.
43. S. Consta. "Understanding the stability of non-covalent complexes of macromolecules in charged droplets by molecular simulations", 21st International Mass Spectrometry Conference, Toronto, Canada, August, 2016. 103 speakers among approximately 1500 participants; 30-min talks were allotted by competition to a small percentage of participants. **International Conference**.
44. S. Consta. "Dissociation rate and mechanisms of protein complexes in solution", 21st International Mass Spectrometry Conference, Toronto, Canada, August, 2016. As in item 4, 20-min talks were allotted by competition to a small percentage of participants. **International Conference**.
45. S. Consta. "Star morphologies of charged droplets beyond the Rayleigh limit", Canadian Symposium on Theoretical and Computational Chemistry (CSTCC) Regina, Saskatoon, July, 2016. **Invited Presentation, National Conference**.
46. S. Consta. "Macroion-induced disintegration of charged droplets beyond the conventional mechanisms", 21st International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI) UBC, Vancouver, Canada, July, 2016. **Plenary Speaker, International Conference**.
47. S. Consta. "Droplet acidity and chemical reactivity" Oral presentation in the CECAM workshop on the topic of "Computational methods for multiply-charged droplets", CECAM-HQ-EPFL, Lausanne, Switzerland, July, 2016 (replacing one of the invited speakers who could not be present). **International Conference**.
48. S. Consta. "Toward the understanding of the stability of non-covalent complexes of macromolecules in charged droplets", Michael Barber Center for Collaborative Mass Spectrometry, University of Manchester, May 16, 2016 (Presentation in the group of Prof. Perdida Barran).
49. S. Consta. "When droplets become stars: charged droplets beyond Rayleigh instability", April 21, 2016 Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany.
50. S. Consta. "Macromolecular ion-solvent interactions in charged droplets" in the Session of "Recent Advances in Dynamics of Confined Liquids", Pacifichem 2015, Hawaii, US, December 20, 2015. **International Conference**
51. S. Consta. "Toward the understanding of the stability of non-covalent complexes of macromolecules in charged droplets", PNNL, October 12, 2015.
52. S. Consta. "The Unique Physical Chemistry of Charged Droplets", Plenary Lecture at the Women in Physics Canada (WIPC) 2015 Conference, University of Toronto, July 30-August 1 , 2015. **National Conference** The presentation was for approximately 1.5 hours. In the first 45-50 min I presented my research (science part) and in the rest of the time I presented my personal view on how to balance professional and personal life in science

and answered questions from the audience.
53. S. Consta. "Stability of charged liquid droplets" Wales group, Department of Chemistry, University of Cambridge, UK, June 5, 2015.
54. S. Consta. "Modelling of charging mechanisms and desolvation of macromolecules in droplets", Department of Chemistry, Durham, UK, May 13, 2015.
55. S. Consta. "Molecular modelling of the ejection mechanisms of macromolecules from charged nanodroplets", Department of Chemistry, King's College, London, UK, April 29, 2015.
56. S. Consta. April 2015. Presentation in the Lucy Cavendish College, where I was a member. I had to cancel the presentation because of illness of a family member.
57. S. Consta. Theoretical Chemistry Informal Seminars, Department of Chemistry, University of Cambridge, November 21, 2014. (Even though the seminars are called "informal", these are formal theoretical chemistry seminars.)
58. S. Consta. "Molecular modelling of the ejection mechanisms of macromolecules from charged nanodroplets" Group Meeting Research Seminar, Dame C. Robinson group, Department of Chemistry, University of Oxford, October 3rd, 2014.
59. S. Consta. "The unique chemistry of charged systems" Group meeting research seminar, group of Prof. Daan Frenkel, Department of Chemistry, University of Cambridge, September 4, 2014.
60. S. Consta. "Molecular modeling of the ejection mechanisms of macromolecules from charged nanodroplets" American Chemical Society (ACS), Analytical Chemistry Divisions, San Francisco (August 10–14, 2014). **International Conference**
61. S. Consta. "Charge-induced instabilities in droplets containing charged macromolecules" Invited talk for "Hot topic" presentation in the Gordon Research Conference (GRC) Molecular and Ionic Clusters: Structure and Dynamics of Isolated Particles: From Small Clusters to Atmospheric Aerosols, Renaissance Tuscany Il Ciocco Resort Lucca (Barga), Italy (April 27-May 2nd, 2014). **International Conference**
62. S. Consta. "Classification of the ejection mechanisms of charged macromolecules from liquid droplets", Seminar in the Department of Chemistry, University of Durham, April 25th, 2014.
63. S. Consta. "Classification of the ejection mechanisms of charged macromolecules from liquid droplets", Informal seminar in the Department of Mechanical Engineering, Yale University, April 1st, 2014.
64. S. Consta. "Ejection mechanisms of macroions from droplets", Chemical Physics Theory Group meetings, Dept. of Chemistry, University of Toronto (January 7, 2014, research and recruiting talk).
65. S. Consta. "Ejection mechanisms of macroions from droplets", Dept. of Chemistry, University of Alberta (November 14, 2013, research and recruiting talk).
66. S. Consta. "Escape Mechanisms of Charged Macromolecules from Droplets", Dept. of Chemistry, University of Saskatchewan (October 8, 2013).
67. S. Consta. "Unraveling the role of solvent- macromolecule interactions in determining the conformations of macromolecules in bulk, droplet and vacuum environments" Applied Mathematics, Modelling and Computational Science (AMMCS) Waterloo, August 28-30, 2013 (August 29, 2013). **International conference**
68. S. Consta. "Conformations of macromolecules in bulk vs. droplet environment" Pacific Northwest National Laboratory (PNNL), August 26, 2013.
69. S. Consta. "Unraveling the escape of macroions from droplets by theory and simulations" Invited talk for "Hot topic" presentation in Gaseous Ions: Structures, Energetics & Reactions Gordon Research Conference (GRC), Galveston, Texas, US (Feb. 24-March 1st, 2013). **International Conference**
70. S. Consta. "Ejection Mechanisms of Charge Macromolecules in Droplets" Seminar in the Department of Physics and Astronomy, UWO, London (January 24, 2013).
71. S. Consta. "Computer simulations of complex systems" Graduate Seminar in Chemical and Biochemical Engineering, UWO, London (December 5, 2012).
72. S. Consta. "Conformational changes of charged PEG in bulk and droplet environments", LANXESS, London (June 8, 2012).
73. S. Consta. "Release mechanisms of macroions from liquid charged nanodroplets", SCIEX-AB, Toronto (April 30, 2012).
74. S. Consta. "Ion transfer in Nanodroplets containing Excess Charge" Dept. of Chemistry, Brock University, St. Catharines, Canada (September 23, 2011).
75. S. Consta. "Ion transfer in Highly Charged Nanodroplets" Dept. of Chemistry, University of Western Ontario, London, Canada (Feb. 2nd, 2011).

76. S. Consta. Accepted invitation for the Theoretical Chemistry Conference, August 2007, St. John's **National Conference**. I could not attend because of maternity leave.
77. S. Consta. During my sabbatical leave a number of talks were presented at
    - ITE-FORTH, Patra, Greece (Feb. 2006);
    - Technical University of Athens, Dept. of Chemical Engineering, Athens, Greece (Feb. 2006);
    - Technical University of Munich, Dept. of Chemistry, Munich, Germany (April 2006);
    - National Hellenic Research Foundation (NHRF) (May 4, 2006);
    - Department of Physics, University of Vienna, Austria (May 10, 2006);
78. S. Consta. "Ion dynamics in aqueous droplets". Dept. of Chemistry, University of Dalhousie, Halifax, Canada (Sept. 1st, 2005).
79. S. Consta. Invited talk in the Canadian Society for Chemistry Conference (CSC), May 2005, Saskatoon. **National Conference**
80. S. Consta. Accepted invitation for the symposium "Classical and Quantum Statistical Mechanics Studies of Solvation" (ACS, Division of Physical and Theoretical Chemistry), PACIFICHEM 2005, Honolulu, Hawaii, Dec. 15-20, 2005. Unable to be present because of illness due to car accident. **International Conference**
81. S. Consta. "Reactive processes in charged systems". Northwestern National Lab, Richland, USA. (December, 2004)
82. S. Consta. "Fragmentation processes of aqueous clusters containing ionic species". Centre d'Etudes de Chimie Metallurgique, Vitry-dur-Seine, Paris France. (January 7, 2003) Talk was cancelled because of unexpected illness of the speaker.
83. S. Consta. "Fragmentation reactions of charged aqueous clusters". Physical Chemistry Seminar, Department of Chemistry, Queen's University, Kingston, (February 4, 2002).
84. S. Consta. "Computer Modeling of highly charged nanodroplets". Canadian symposium on Theoretical Chemistry, Ottawa (2001). Invited Oral Poster presentation. **International Conference**
85. S. Consta. "Fragmentation Reactions of charged clusters". Seminar in FORTH (Research Institute), Crete, Greece (2001) .
86. S. Consta. "Ionization reactions of salts in mesoscopic water clusters". Seminar in the Department of Applied Mathematics, University of Western Ontario, London (2001).
87. S. Consta. "Methodologies to study Reaction mechanisms". Department of Chemistry, University of Ioannina, Ioannina, Greece (2001).
88. S. Consta. "Dynamics of water condensation". Physical Chemistry Seminar in the Department of Chemistry, University of Toronto, Toronto (1999).
89. S. Consta. "Look-ahead" Configurational Bias Monte Carlo Scheme for Polymer systems. Talk in the conference "Algorithms for Simulation Complex Molecular Systems" in CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lyon, France (1998). **International Conference**

Contributed Talks and Poster Presentations by S. Consta

1. S. Consta, V. Kwan, and H. Nguyen. Poster presentation entitled "Chemistry in supercooled droplets", Gordon Conference on the Chemistry and Physics of Liquids, Holderness, NH, US, August 3-9, 2025. **International Conference**
2. S. Consta, M. In-Oh, and H. Nguyen. Poster presentation entitled "Determining the protein protonation state in evaporating electrosprayed droplets: A multi-scale computational approach applicable from the nano-scaled to micro-scaled droplets", Chemical Biophysics Symposium, University of Toronto, May 9-11, 2025. **International Conference**
3. S. Consta. Oral presentation entitled "Identifying the variety of charging mechanisms of macromolecules in droplet-based ionization methods coupled to mass spectrometry", CSC, Session: Ion Solvation, Winnipeg, June 3rd 2024. **National Conference**.
4. S. Consta, "Molecular Modelling of Ion Transfer at Interfaces", presentation in the group meeting of the Electrochemistry/Corrosion groups in the Dept. of Chemistry, December 4, 2023.
5. S. Consta, Chemical Physics Symposium, University of Waterloo, November, 2023.

6. S. Consta "Atomistic modelling provides direct observation of Rayleigh jets in charged droplets". Oral presentation in XIXth International Congress on Rheology (ICR2023), July 29-August 4, 2023, Athens, Greece. **International Conference**
7. S. Consta, Title: Evolution of the charge state of macroions from the bulk solution to the vapor state - Insight from computational modelling. Oral presentation in Mass Spectrometry symposium, IUPAC/Canadian Chemistry Conference and Exhibition (CCCE), August 13-20, 2021 (virtual). **National Conference**
8. S. Consta, Poster presentation in CAMBR, UWO, June 17, 2021. **Institutional Conference**
9. S. Consta, Title: Modelling of macroion-droplet interactions - formation of "star"-shaped droplets. Pacifichem 2021; Symposium: Interfacial Phenomena for Bubbles, Droplets, Films and Soft Matter (December 2021). **International Conference**
10. S. Consta, Title: Structure and dynamics of curved interfaces. Pacifichem 2021; Symposium: Advanced Understanding of Soft Interfaces at the Molecular-Scale (December 2021). **International Conference**
11. S. Consta Title: Will droplet be the "new beaker" of chemistry? Insight from theory on the effect of charge in droplet structure and reactivity. Special Seminar in Lawrence Berkeley National Laboratory (Host: Dr. Kevin Wilson), Feb. 15, 2021.
12. S. Consta Title: Bridging electrostatic properties and surface tension between nanoscopic and microscopic highly charged droplets Session: (PTC Division) - Advances in physical, theoretical, and computational chemistry, Canadian Society for Chemistry (CSC), Winnepeg MB, May 24-28, 2020 Oral presentation (conference was cancelled due to the pandemic). **National Conference**
13. S. Consta Title: Protein complex dynamics in bulk solution and droplets Session: (PTC/BM Divisions) - Biomolecular dynamics: experimental and computational advances, Canadian Society for Chemistry (CSC), Winnepeg MB, May 24-28, 2020 Oral presentation (conference was cancelled due to the pandemic). **National Conference**
14. S. Consta Molecular characterization of the surface excess charge layer in droplets with simple ions and macroions Session: (PTC Division) - Poster presentation Canadian Society for Chemistry (CSC), Winnepeg MB, May 24-28, 2020 (conference was cancelled due to the pandemic). **National Conference**
15. S. Consta. "Extrusion mechanisms of macroions from droplets", Analytical Chemistry Division, American Chemical Society (ACS) Meeting, San Diego, August 25-29, 2019. **International Conference**
16. S. Consta. "Computational modelling of the equilibrium constant of non-covalent complexes of proteins in droplets and bulk solution", Advances in Physical, Theoretical and Computational Chemistry (General Session), Canadian Society for Chemistry (CSC), Quebec City, June 3-7, 2019. **International Conference**
17. S. Consta. "Macroion-Solvent Interactions in Charged Droplets", Analytical Platforms and Functional Materials, Canadian Society for Chemistry (CSC), Quebec City, June 3-7, 2019. **International Conference**
18. S. Consta. Presentation in the group meeting of Prof. E. Kaxiras, April 3rd, 2019, John A. Paulson School Of Engineering end Applied Sciences, Harvard.
19. S. Consta. Poster presentation in Gaseous Ions: Structures, Energetics and Reactions Gordon Research Conference, February 17-22, 2019 (Ventura, California). **International Conference**
20. S. Consta. Poster "Stability of of weak protein-protein interactions in charged aqueous droplet" American Society for Mass Spectrometry, San Diego, US June 5-June 8, 2018. In addition to the poster I also prepared proceedings, submitted to the ASMS. **International Conference**
21. S. Consta. "What factors determine the stability of weak protein-protein interactions in a charged aqueous droplet?" in the session of Analytical Mass Spectrometry, Canadian Society for Chemistry Conference (CSC) Edmonton, May 27-June 1st, 2018. **International Conference**
22. S. Consta. "Stability of protein complexes in droplets", Poster, Sanibel Conference, Jan. 25-29, 2018, St. Petersburg, FL, US. **International Conference**
23. S. Consta. " Modelling of the Rate and Mechanism of Dissociation of non-Covalent Complexes in a Charged Aqueous Droplet" Oral Contributing Presentation in the Analytical Chemistry Session, Canadian Society for

Chemistry Conference, May 28-June 1, 2017, Toronto, Canada. **National Conference**

24. S. Consta. "Characterization of the structure of the "star"-shaped droplets", Presentation in the group meeting of Prof. D. Frenkel, Dept. of Chemistry, University of Cambridge, UK, November 3, 2016.
25. S. Consta. Poster presentation with title "Star formation of charged droplets" Soft Matter - Theoretical and Industrial Challenges Celebrating the Pioneering Work of Sir Sam Edwards, Isaac Newton Institute, Cambridge, UK, September 7 - 9, 2016. **International Conference**
26. S. Consta, M. Sharawy. Poster presentation with title "How do non-covalent complexes dissociate? A case study of the double stranded DNA in an aqueous droplet" in European Molecular Liquids Group (EMLG) and the Japanese Molecular Liquids Group (JMLG), Sept. 11-16, 2016, Chania, Greece **International Conference**
27. Mahmoud Sharawy and S. Consta. Poster presentation, Regina July 10-15, 2016 **National Conference**
28. S. Consta. "Droplet acidity and chemical reactivity" Oral presentation in the CECAM workshop on the topic of "Computational methods for multiply-charged droplets", CECAM-HQ-EPFL, Lausanne, Switzerland, July 6-8, 2016 (replacing one of the invited speakers who could not be present). **International Conference**
29. S. Consta. "Characterization of the "star"-shaped droplets", Presentation in Wales group, Department of Chemistry, University of Cambridge, UK, June 7, 2016.
30. S. Consta. "Continuum modelling of the "star"-shaped droplets", Presentation in Frenkel group, Department of Chemistry, University of Cambridge, UK, May 26, 2016.
31. M. Sharawy and S. Consta. "Stability of non-covalent complexes of macromolecules in charged droplets" 2015 Symposium of Chemical Physics, University of Waterloo, November 6, 2015. **International Conference**
32. S. Consta. "Star morphologies of charged droplets", Research seminar in the group meeting of Prof. D. Frenkel's group, Department of Chemistry, University of Cambridge, UK, June 4, 2015.
33. S. Consta. and D. Frenkel "Counter-intuitive Shapes of Charged Droplets: Stars, Necklaces and Extruding Tails", Poster in the Open Day in the Department of Chemistry, University of Cambridge, UK, October 24, 2014. **Institutional Conference**
34. S. Consta. and Falana Sheriff "Charge-induced droplet morphologies by macromolecular complexes", Oral presentation in the QSAR meeting, Cambridge, Sept. 30, 2014. **National Meeting**
35. S. Consta. "Macromolecule-ion interactions in bulk solution and droplet environment", Poster at the Gordon Conference "Water and Aqueous Solutions", Holderness School, NH, July 27-August 1st, 2014. **International Conference**
36. S. Consta. "Macromolecule-ion interactions in bulk solution and droplet environment", Poster at the 26th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Montreal, July 7-11, 2014. **International Conference**
37. S. Consta. "Macromolecule-ion interactions in bulk solution and droplet environment", Poster in the Soochow University workshop in the framework of the collaboration between UWO and Soochow University, May 5-8, 2014.
38. S. Consta. "Charge-induced instabilities of droplets containing charged macromolecules" Poster presentation in the Gordon Research Conference (GRC) Structure and Dynamics of Isolated Particles: From Small Clusters to Atmospheric Aerosols, Renaissance Tuscany Il Ciocco Resort Lucca (Barga), Italy (April 27-May 2nd, 2014). **International Conference**
39. S. Consta. Poster presentation with title "Escape mechanisms of macroions from droplets studied by theory and simulations" in Gaseous Ions: Structures, Energetics & Reactions Gordon Research Conference (GRC), Galveston, Texas, US (Feb. 24-March 1st, 2013). **International Conference**
40. S. Consta. Oral presentation with title "The phase diagram of the ejection of a charged macromolecule from a droplet", oral presentation in the 2012 Symposium on Chemical Physics, University of Waterloo, November 2-4, 2012. **National Conference**
41. **S. Consta**. Oral presentation with title "Mechanisms of phase transformations of TiO_2 nanotubes and nanorods", Canadian Materials Science Conference (London, Ontario), Session:Nanomaterials, June 5-8, 2012.

National Conference

42. S. Consta. Oral presentation with title "Analytical and simulation modelling of release of macroions from droplets", CSC (Calgary, Alberta), Session: Multi-scale Bio/Physical/Chemical Modelling, May 28, 2012. **National Conference**
43. S. Consta. Oral presentation with title "Manifestations of Rayleigh instability in droplets with macroions", CSC (Calgary, Alberta), Session: Physical/Theoretical Mass Spectrometry, May 27, 2012. **National Conference**
44. **S. Consta**. Poster presentation with title "Ion transfer in nanodroplets containing excess charge", Gordon Conference (Ventura, California), Jan. 29-Feb. 3, 2012. **International Conference**
45. S. Consta. Oral presentation with title "Ion transfer mechanisms in charged nanodroplets", 2011 Symposium on Chemical Physics, University of Waterloo, November 4-6, 2011. **National Conference**
46. S. Consta. Oral presentation with title "Proton transfer in charged nanodroplets", 2011 Symposium on Chemical Physics, University of Western Ontario, March 9-11, 2011.
47. **S. Consta**. Oral presentation with title "Effect of charged environment in proton transfer in aminoacids and peptides", CSC, Montreal, June 5-9, 2011 (The presentation was on June 9, 2011). **National Conference**
48. S. Consta. Oral presentation with title "Effect of charged environment in proton transfer from peptides", CSC, Toronto, May 30-June 2nd, 2010.
49. Jun Kyung Chung and S. Consta. Poster with title "Charge induced transitions of PEG-(Na+)n in vacuum and aqueous droplets", CSC, Toronto, May 30-June 2nd, 2010. **National Conference**
50. S. Consta. Poster with title "Fragmentation processes in charged droplets containing macroions" presented in the 7th Canadian Computational Chemistry Conference, Halifax, July 20-24, 2009. **International Conference**
51. S. Consta. Oral presentation with title "Manifestation of Rayleigh instability in charged droplets containing macroions", CSC, Hamilton, May 30-June 3rd, 2009. **National Conference**
52. S. Consta. Organizer of the symposium: Classical and quantum approaches for rare event dynamics. *39th Canadian Society for Chemistry Conference*, London, Ont., May 29-June 1, 2004. **National Conference**
53. S. Consta. "Fragmentation processes of ultra-fine aqueous droplets with ions and glucose" **National Conference** Talk in *39th IUPAC Congress and Conference of the Canadian Society for Chemistry*, Ottawa (Aug. 10-15, 2003). **National Conference**
54. S. Consta, K. Mainer. "Fragmentation processes of ultra-fine aqueous droplets" Poster in *39th IUPAC Congress and Conference of the Canadian Society for Chemistry*, Ottawa (Aug. 10-15, 2003). **National Conference**
55. A. Stavrakoudis and S. Consta. "Structure of Alanine Dipeptide in mixture of solvents." Poster in *Chemical Biophysics Symposium*, Toronto (April 2002). **National Conference**
56. S. Consta. "Disintegration of highly charged nanoscale droplets." Talk in the Centre of Chemical Physics, University of Western Ontario, London (2001).
57. S. Consta. "Dynamics of Coulomb Explosion of clusters." , Talk in Physical Chemistry Session, *Canadian Society for Chemistry*, Calgary, Alberta (2000). **National Conference**
58. S. Consta. "Dynamics of vapour-liquid phase transition of water." Poster in conference of Physical Chemistry, Luteren, The Netherlands (1999).
59. S. Consta. "Biased Monte Carlo schemes for polymer systems." Poster in conference of Physical Chemistry, Luteren, The Netherlands (1998). **National Conference**
60. Styliani Consta. "Reactions in clusters." Talk in AMOLF, Amsterdam, The Netherlands (1996).
61. S. Consta "Proton transfer in mesoscopic, molecular clusters." Poster in 12th Canadian Symposium on Theoretical Chemistry, Fredericton, New Brunswick (1995). **National Conference**

Talks and Poster Presentations of Students and Postdoctoral Fellows

The presenter is underlined. In all the posters and oral presentations SC is included as a co-presenter.

1. Marko Voronych, S. Consta*, Poster entitles "Molecular modelling assessment of Taylor cone predictions of analytical theory", University of Waterloo Symposium on Chemical Physics, November 7-9, 2025.

2. Jihong Shi, Han Nguyen, Mateo Pescador Arboleda, S. Consta*, Poster entitled "From sphere to cones: Structural instabilities and acidity at conical regions in trivalent metal ion nano-clusters", Lennard-Jones Centre-CECAM Meeting 2025, Cambridge, UK September 1-5, 2025. **International Conference**.
3. Han Nguyen and S. Consta. Poster presentation entitled "Chemical reactivity in supercooled droplets", CSC, Ottawa, June 15-19, 2025. **National Conference**.
4. Margaret Petrova and S. Consta. Oral presentation entitled "Molecular Modelling of the Structural Distortions in Ion-Doped Hexagonal Ice" in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), University of Guelph, March 29, 2025. **Regional Conference**.
5. Han Nguyen and S. Consta. Poster presentation entitled "Simulation Methods for Evaporating Electrosprayed Droplets", Chemical Physics Symposium, Waterloo, November 8-10, 2024. **National Conference**.
6. Margaret Petrova and S. Consta. Poster presentation entitled "Ion-Water Interactions in Supercooled Droplets", Chemical Physics Symposium, Waterloo, November 8-10, 2024. **National Conference**.
7. Han Nguyen and S. Consta. Oral presentation entitled "Computational methods to study the solvation of macroions in an evaporating droplet", CSC, Session: Ion Solvation, Winnipeg, June 3rd 2024. **National Conference**.
8. Amber Wu and S. Consta. Poster presentation entitled "On the Origins of Life - Modelling the initial stages of complex coacervate droplet formation", Chemical Biophysics Symposium, University of Toronto, April 2024. **National Conference**.
9. Alan Dziuba Oral presentation entitled "Interactions of protein with water at supercooling" in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), The University of Western Ontario (March 2024). **Regional Conference**.
10. Amber Wu and S. Consta. 3-min Talk and Poster presentation entitled "On the Origins of Life - Modelling the initial stages of complex coacervate droplet formation" in the Origins of Life Donostia Meeting (OLDM'23), Donostia-San Sebastian, Spain, October 2-4, 2023. **International Conference**.
11. Amber Wu and S. Consta. Poster presentation entitled "On the Origins of Life - Modelling the initial stages of complex coacervate droplet formation" in the Biennial European Astrobiology Conference (BEACON), Canary Islands, May 2023. **International Conference**.
12. Nicholas Bainbridge "Atomistic Modelling of Weak-Protein Interactions in Solution", Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Trent University, March 25, 2023. **Regional Conference**.
13. Amber Wu Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Trent University, March 25, 2023. **Regional Conference**
14. V. Kwan Poster presentation in the "Water and Aqueous Solutions" Gordon Conference (Water on Multiple Length Scales from the Molecular Level to the Global Hydrosphere), Holderness School, NH, July 23, 2022-July 29, 2022. **International Conference**
15. Farshad Esmaeilian Oral presentation in CSC, June 13-17, 2022, Calgary. **National Conference**
16. Remi Sampaleanu Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), University of Toronto (March 26th, 2022, virtual). **Regional Conference**
17. Garvin Tran Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), University of Toronto (March 26th, 2022, virtual). **Regional Conference**
18. Emmeline Rittau Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), University of Toronto (March 26th, 2022, virtual). **Regional Conference**
19. Shoubhik R. Maiti and S. Consta, Western Student Research Conference, "Salt Rejection in Supercooled Aqueous Droplets-Implications in Atmospheric Aerosol Chemistry and Mass Spectrometry", September 19, 2021 (virtual, Institutional conference).
20. V. Kwan and S. Consta, Title: Computational insight into the droplet-ion interactions. Oral presentation in symposium "Chemistry in small volumes", IUPAC/Canadian Chemistry Conference and Exhibition (CCCE), Aug.

13-20, 2021 (virtual).

21. Wenhan Zhang "Study of Cholera Toxin Assembly Mechanism by Molecular Dynamics" Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), McMaster (March 20th, 2021, virtual). **Regional Conference**
22. Nadreen Elsawish Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Ryerson University (June 15th, 2020, virtual). Award received: Outstanding Oral Presentation Award in Physical, Theoretical, & Computational Chemistry. **Regional Conference**
23. David Laur Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Ryerson University (June 15th, 2020, virtual).
24. V. Kwan and S. Consta. Oral presentation Applied Mathematics, Modelling and Computational Science (AMMCS), Waterloo, August 18-23, 2019. **International Conference**
25. V. Kwan and S. Consta. Oral presentation in the Canadian Society for Chemistry (CSC), Quebec City, June 3-7, 2019. **National Conference**
26. J. Chen and S. Consta. Poster presentation in the Canadian Society for Chemistry (CSC), Quebec City, June 3-7, 2019. **International Conference**
27. A. Luong and S. Consta. Poster presentation in the Chemical Biophysics symposium, Toronto, May 3-5, 2019 **International Conference**
28. A. Luong Oral and poster presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), University of Toronto, Scarborough campus (March 30th, 2019). **Regional Conference**
29. V. Kwan Oral presentation, Department of Chemistry, Rits-UWO workshop (organized by Prof. M. Stillman) University of Western Ontario, February 26, 2019. **Institutional Conference**
30. V. Kwan and S. Consta, Poster in the Water and Aqueous Solutions Gordon Conference, Holderness School in Holderness, NH, United States, (July 22-27, 2018). **International Conference**
31. M. In Oh and S. Consta Oral presentation in the Chemistry Graduate Student Symposium, University of Buffalo (May 21st-23rd, 2018). **Institutional Conference**
32. R. Szukalo and S. Consta Oral presentation in the Chemistry Graduate Student Symposium, University of Buffalo (May 21st-23rd, 2018). **Institutional Conference**
33. R. Szukalo Oral presentation in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Wilfrid Laurier University (March 24, 2018). **Regional Conference**
34. C. Graham and S. Consta, 2 min oral presentation and poster entitled "Ionization reactions of complexes of ions in solution", Berkeley Statistical Mechanics Meeting, University of California at Berkeley, US, January 12-14, 2018. **International Conference**
35. Myong In Oh and S. Consta, "Stability of a protein complex in an evaporating droplet", Berkeley Statistical Mechanics Meeting, University of California at Berkeley, US, January 12-14, 2018. **International Conference**
36. V. Kwan, M. In Oh and S. Consta, "From stars to assembly of nanoparticles", poster presentation, Chemical Physics Symposium, Waterloo, Nov. 3-5, 2017. **International Conference**
37. C. Graham and S. Consta, poster presentation, Chemical Physics Symposium, Waterloo, Nov. 3-5, 2017. **International Conference**
38. C. Graham, oral presentation Applied Mathematics, Modelling and Computational Science (AMMCS), Waterloo, August 20-25, 2017. **International Conference**
39. M. Sharawy, oral presentation Applied Mathematics, Modelling and Computational Science (AMMCS), Waterloo, August 20-25, 2017. **International Conference**
40. M. In Oh, oral presentation Applied Mathematics, Modelling and Computational Science (AMMCS), Waterloo, August 20-25, 2017. **International Conference**
41. M. In Oh, oral presentation CSC2017, Toronto, May 28-June 1st, 2017 **International Conference**
42. Rachel McCormack, S. Consta. in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC) in York University, March 18, 2017. **Regional Conference**

43. M. In Oh, S. Consta. Poster presentation in Graduate Student and Research Gordon Conference, Gaseous Ions: Structure, Energetics and Reactions; Gas-Phase Ion Chemistry: From Fundamentals to Applications, Ventura, US, February, 2017. **International Conference**
44. M. In Oh, S. Consta. Oral presentation in the Chemical Physics Symposium, University of Waterloo, November 6, 2016. **International Conference**
45. M. In Oh, S. Consta. Poster presentation, CECAM-HQ-EPFL, Lausanne, Switzerland, July 6-8, 2016. **International Conference**
46. M. Sharawy, S. Consta. "Effect of counterions in the charging of macromolecules and complexes in droplets" Poster presentation, CECAM-HQ-EPFL, Lausanne, Switzerland, July 6-8, 2016. **International Conference**
47. S. Soltani, S. Consta. Poster presentation, CECAM-HQ-EPFL, Lausanne, Switzerland, July 6-8, 2016. **International Conference**
48. A. Tumarov, S. Consta. "Characterizing star morphologies of charged droplets", Western Student Research Conference, March 19, 2016. **Institutional Conference**
49. M. In Oh, S. Consta. Research talk in the group meeting of Prof. D. Frenkel, Department of Chemistry, University of Cambridge, UK, March 10, 2016.
50. M. In Oh, S. Consta. Review on colloid science, talk in the group meeting of Prof. D. Frenkel, Department of Chemistry, University of Cambridge, UK, March 16, 2016.
51. M. In Oh, S. Consta. "Effect of confinement in the conformations of of macromolecules in droplets" Poster at Chemical Physics Symposium, Waterloo, Nov. 7, 2015. **International Conference**
52. M. Paliy, S. Consta and J. Yang. Oral presentation on "Interactions between carbon nanoparticles and fragmentation of a droplet of organic solvent" Applied Mathematics, Modelling and Computational Science Congress (AMMCS-CAIMS), Waterloo, Ontario, June 6, 2015. **International Conference**
53. S. Soltani, S. Consta. Oral presentation on "Effect of the droplet confinement in the conformations of macromolecules" Applied Mathematics, Modelling and Computational Science (AMMCS-CAIMS) Congress, Waterloo, Ontario, June 6, 2015. **International Conference**
54. Mahmoud Sharaway and S. Consta. Oral presentation on "The effect of counter ions on the release mechanisms of charged macromolecules from nanodroplets" Applied Mathematics, Modelling and Computational Science (AMMCS-CAIMS) Congress, Waterloo, Ontario, June 6, 2015. **International Conference**
55. F. Sheriff and S. Consta. Oral presentation on "Interactions of Macromolecular Complexes in Charged Aqueous Nanodrops" Applied Mathematics, Modelling and Computational Science (AMMCS-CAIMS) Congress, Waterloo, Ontario, June 6, 2015. **International Conference**
56. Myong Oh and S. Consta. Oral presentation on "Effect of Solvent on Solvation and Sodiation Mechanisms of Poly(ethylene glycol) in Droplets" Applied Mathematics, Modelling and Computational Science (AMMCS-CAIMS) Congress, Waterloo, Ontario, June 6, 2015. **International Conference**
57. Nicole Maione, Oral presentation: "Treatment of Electrostatic Interactions in Molecular Simulations" in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Physical Chemistry Session, March 21st, 2015, University of Toronto, Mississauga Campus. **Regional Conference**
58. Myong Oh and S. Consta, "Effect of solvent in the charging mechanism of Poly(ethylene glycol) in charged droplets" Poster at Chemical Physics Symposium, Waterloo, Nov. 9, 2014. **International Conference**
59. Myong Oh and S. Consta "Release Mechanism of a Poly(ethylene glycol) from a Highly Charged Aqueous Droplet" at Poster at the 26th Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Montreal, July 7-11, 2014. **International Conference**
60. S. Soltani and S. Consta, Poster presentation "Solvation of Poly(ethylene glycol) in Aqueous Nanodroplets" (May 3rd, 2014) at the Chemical Biophysics Symposium, University of Toronto, May 2nd-May 4, 2014. **International Conference**
61. F. Sheriff and S. Consta, Poster presentation "Interactions of Macromolecular Complexes in Charged Aqueous Nanodroplets" (May 3rd, 2014) at the Chemical Biophysics Symposium, University of Toronto, May 2nd-May

4, 2014. **International Conference**

62. Filipe de Souza, Oral presentation "Effect of charge distribution on the stability of droplets" *2nd Prize* in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Analytical Chemistry Session, March 29, 2014, University of Windsor. **Regional Conference**
63. Falana Sheriff, Oral presentation: "Interactions of complexes of macromolecules in charged nanodroplets" (*1st Prize* in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), Physical Chemistry Session, March 29, 2014, University of Windsor. **Regional Conference**
64. Myong Oh and S. Consta "Release Mechanism of a Poly(ethylene glycol) from a Highly Charged Aqueous Droplet" at Chemical Physics Symposium, Waterloo, Nov. 2, 2013. **International Conference**
65. Mahmoud Sharaway and S. Consta "The effect of counter ions on the release mechanisms of charged macromolecules from nanodroplets" at Chemical Physics Symposium, Waterloo, Nov. 2, 2013. **International Conference**
66. F. Sheriff and S. Consta. Poster presentation with title "Effect of counterions in the escape of charged PEG from nanodroplets" at Midwestern Symposium on Undergraduate Research in Chemistry", Michigan, Oct. 5, 2013. **International Conference**
67. Matthew Turnbull, Oral presentation: "Charge-Induced Instability in Droplets with Charged Macromolecular Complexes – Study of siRNA in Aqueous Droplets" in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC), McMaster University, March 30, 2013. **Regional Conference**
68. M. Turnbull and S. Consta. Poster presentation with title "Ejection mechanisms of a charged macromolecule from a droplet", in the 2012 Symposium on Chemical Physics, University of Waterloo, November 2-4, 2012. **International Conference**
69. Z. Hui and S. Consta. Poster presentation with title "Conformational changes of molecules inside NaY zeolites", Canadian Society for Chemistry (CSC), May 30-June 3rd, 2009, Hamilton. **International Conference**
70. E. Lam and S. Consta. "Sampling of reactive paths for computations of reaction rates in the condensed phase". Poster presentation in *39th Canadian Society for Chemistry Conference*, London, Ont., May 29-June 1, 2004. **International Conference**
71. S. Lam, Y. Liu and S. Consta. "Properties of $(NH_3)(H_2O)_n$ (n=1-4) clusters on the surface of a carbon nanotube and confinement effects on the structure of a fluid". Poster presentation in *39th Canadian Society for Chemistry Conference*, London, Ont., May 29-June 1, 2004. **International Conference**
72. M. Paliy, O. Braun and S. Consta. " Ordering of a thin lubricant film due to sliding". Oral poster presentation in the *39th Canadian Society for Chemistry Conference*, London, Ont. May 29-June 1, 2004. **International Conference**
73. Y. Liu and S. Consta. "Dissociation of water inside carbon nanotubes". Oral poster presentation in the *39th Canadian Society for Chemistry Conference*, London, Ont., May 29-June 1, 2004.
74. S. Consta. "Fragmentation processes of ultra-fine aqueous droplets with ions and glucose" Talk in *39th IUPAC Congress and Conference of the Canadian Society for Chemistry*, Ottawa (Aug. 10-15, 2003). **International Conference**
75. M. Paliy, S. Consta. "Empirical Potential Model for the Oxidation of Silicon" Poster in *39th IUPAC Congress and Conference of the Canadian Society for Chemistry*, Ottawa (Aug. 10-15, 2003). **International Conference**
76. Y. Liu, R. O. Jones, Xinluo Zhao, Yoshinori Ando, S. Consta. Carbon species confined inside carbon nanotubes: A DFT study. Poster in Canadian Computational Chemistry Conference (CCCC5), Toronto (July 2003). **International Conference**
77. F. Ogeer, S. Consta and R. H. Lipson. Structure of small clusters of Methanol and Ethanol Mixtures and their cluster size Distributions. Poster in Canadian Computational Chemistry Conference (CCCC5), Toronto (July 2003).
78. W. Novak, S. Consta. Crystallization of NaCl in mesoscopic aqueous clusters. Poster in the *American Conference of Theoretical Chemistry*, Seven Springs, PA (July 13, 2002) **International Conference**

79. A number of other posters have been presented by undergraduate and graduate students in the research group at Canadian Computational Chemistry Conference (CCCC5) (Toronto, 2003), IUPAC Congress-CSC (Ottawa, 2003) and SHARC-Net Conference in 'Computer Simulations of Soft and Nano/Meso scale materials', (London, Ont. Aug. 24-26, 2003). The undergraduate students in my lab participate in the annual Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC) and give oral presentations of their research.

Organization of Conferences, Sessions in Conferences, Chair in Sessions

1. S. Consta Co-organizer of the symposium "Biomolecular Dynamics - Experimental and Computational Advances" for the Canadian Society for Chemistry (CSC) Meeting 2022 (Calgary).
2. S. Consta "Interactions and assemblies of proteins" for the Canadian Society for Chemistry (CSC) Meeting 2020 (Winnepeg)- The symposium has been approved, and it also involved other co-organizers (cancelled).
3. S. Consta and Prof. S. S. Xantheas organization of a thee-session symposium on "Chemistry in small volumes" for IUPAC/Canadian Society for Chemistry (CSC) Meeting, Aug. 13-20, 2021 (virtual).
4. S. Consta (principal organizer) Submitted a proposal and approved for a workshop with CAMBR, University of Western Ontario (April 2020) (cancelled)
5. S. Consta . Co-organizer with Prof. R. Bowles of a three-session symposium "Interactions of Macromolecules, Ions, and Colloids in the Condensed Phase: Computational and Experimental Advances" in CSC (Canadian Society for Chemistry) Quebec City, June 3-7, 2019.
6. S. Consta. Co-organizer of a symposium in the ACS Division of Analytical Chemistry ACS Fall National Meeting (August 25 - 29, 2019) in San Diego, CA.
7. S. Consta. Co-organizer with Prof. Gren Patey and Prof. R. Bowles of a symposium on "Challenges in simulations in soft and hard matter", CSC (Canadian Society for Chemistry) 2018, Edmonton, Canada
8. S. Consta. Organizer of a session on "Interactions of Charged Species in Droplets and Bulk" that took place on May 26, 2017 in the CSC 2017, May 28-June 1st, 2017. (sole organizer)
9. S. Consta. Invited to organize computational symposium at the Applied Mathematics, Modelling and Computational Science Congress (AMMCS-CAIMS), Waterloo, Ontario, August, 2017. (sole organizer)
10. S. Consta. Co-applicant in "Computational methods for modelling multiply-charged droplets" CECAM (Centre Européen de Calcul Atomique et Moléculaire), Lausanne, Switzerland, July 6-8, 2016. Other co-applicants: Marie-Pierre Gaigeot (Evry), Mark Miller (Durham), Sotiris Xantheas (PNNL). (successful)
11. S. Consta. Organizer of a session at the Applied Mathematics, Modelling and Computational Science Congress (AMMCS-CAIMS), Waterloo, Ontario, June 6, 2015. (sole organizer)
12. S. Consta. Organizer of the symposium: Classical and quantum approaches for rare event dynamics. *39th Canadian Society for Chemistry Conference*, London, Ont., May 29-June 1, 2004 (**National Conference**).
13. S. Consta. Chairing of sessions in conferences:
    (a) Chairing two sessions in the symposium "Interactions of Macromolecules, Ions, and Colloids in the Condensed Phase: Computational and Experimental Advances" in CSC (Canadian Society for Chemistry) Quebec City, June 3-7, 2019.
    (b) Chair of a session in the Canadian Society for Theoretical and Computational Chemistry, July 15-19, 2018. I had to cancel my participation because of an emergency.
    (c) Session Chair in the CECAM (Centre Européen de Calcul Atomique et Moléculaire) workshop, "Computational methods for modelling multiply-charged droplets", CECAM-HQ-EPFL, Lausanne, Switzerland, July 6-8, 2016.
    (d) Chair of a conference session in the "26th Canadian Symposium of Theoretical and Computational Chemistry", Concordia University, Montreal, July 6-11, 2014;
    (e) International Conference on Nanomaterials 2013, UWO, London, Ontario (August 12-16, 2013);
    (f) Chemical Biophysics Symposium, Toronto (March 19-21, 2004).
    (g) "Canadian Computational Chemistry Conference 5 (CCCC5)", Toronto (July 2003);

TEACHING

My teaching assignments throughout the years can be found at: http://uwo.ca/chem/people/faculty/constas.htm

A. Undergraduate courses

1. CHEM2274a: Thermodynamics and Kinetics (2024, 2025)
2. CHEM4424b: Molecular Structure and Simulation (2024, 2025)
3. CHEM2374a: Thermodynamics (2015, 2018-2023)
4. ES3300 : Environmental Science (I was one of the two co-instructors of the course, which was equally divided between the two co-instructors of the course) (2020, 2021, 2022)
5. CHEM4491: Co-coordinator (two co-coordinators in the course) of the 4th year Honours theses (2013-14, 2019-20, 2020-21)
6. CHEM4444a: Statistical Mechanics and Simulations (1999-2003, 2008-2010, 2012, 2015, 2019, 2021)
7. BIOCHEMISTRY 3383G. This is a research-based course where I supervise 1-2 students during a single term, fall or winter (2021, 2022, 2023)
8. CHEM2384b: Microscopic phenomena (2016, 2017)
9. CHEM3374a: Quantum Mechanics and Spectroscopy (2012, 2013)
10. CHEM4474b: Advanced Quantum Chemistry and Spectroscopy (2011, 2013, 2016)
11. CHEM2214b: Thermodynamics for life science (2001-2004, 2008-2011)
12. CHEM1024a: First Year Chemistry for Engineers (2008, 2009, 2010)
13. SE204b: Basic Science for Software Engineers (2003)

B. Graduate courses offered at Western University

1. Electrostatics in molecular modelling: Electric double layer and charging (Quarter course, forthcoming)
2. Electrostatics of chemical and biochemical systems
3. Applications of Statistical Mechanics: from experiments to computer simulations, CHEM 554y
4. Molecular Dynamics Methods, CHEM9554S (Quarter Course)
5. Advanced Methods in Molecular Simulations/Statistical sampling of rare events in simulations, CHEM9654Q

C. Graduate courses offered at University of California, Irvine

1. "Introduction to Theoretical Methods with Applications to Atmospheric Aerosols", University of California, Irvine, April-June 2023.

C. Training of highly qualified personnel

4th-year theses	NSERC-summer students	summer students	3rd-year research students	MSc	PhD	PDFs	Visiting Professors
42	8	3	3	5	5	9	3

Volunteering Students	Research Internship Students (MITACS)	Exchange Students	High School Students	Work-study Students
13	12	1	1	3

4th year Undergraduate Students' Theses- Principal Supervisor: S. Consta

1. Sept. 2024-April 2025: "The automation of cone angle calculation in "star"-shaped charged droplets", Department of Computer Science (completed).

2. Sept. 2024-April 2025: "Molecular modelling of the structural distortions in ion-doped hexagonal ice", Department of Chemistry (completed). **Awards received while in my lab:** Alumni Gold Medal, Department of Chemistry, UWO. Current position: Student in the Dental School, University of Toronto.
3. Sept. 2023-April 2024: "Hydration patterns on AAV2 Capsid: A molecular dynamics study for enhanced gene therapy vector design", Department of Biochemistry (completed).
4. Sept. 2023-April 2024: "Molecular dynamics of AAV2 in aerosolized environments", Department of Biochemistry (completed).
5. Sept. 2023-April 2024: "Interactions of protein with water at supercooling", Department of Chemistry (completed).
6. Sept. 2022-April 2023: "Solvation of aromatic hydrocarbons in supercooled aqueous droplets", Department of Chemistry (completed).
7. Sept. 2022-April 2023: "Stability of protein complexes in solution", Department of Chemistry (completed).
8. Sept. 2022-April 2023: "Effect of low temperature in the protein interactions", Department of Biochemistry (completed).
9. Sept. 2022-April 2023: "On the Origins of Life - Modelling the initial stages of complex coacervate droplet formation", Medical Biophysics (completed). **Poster award in the Medical Biophysics Symposium** (Institutional). The thesis was one of the 5 winning theses for Western Libraries Undergraduate Research Awards in 2023 competition. Following position: Research assistant, Dept. of Biology, University of Cambridge, UK.
10. Sept. 2021-April 2022: "Intrinsically disordered proteins in supercooled solution", Department of Biochemistry (completed).
11. Sept. 2021-April 2022: "The Mechanism of β-Trypsin and BPTI Encounter Complex Formation in Solution", Department of Biochemistry (completed). Following position: Employed by a bioinformatics company.
12. Sept. 2020-April 2021: "Path Integral Molecular Dynamics of the Proton Transfer Reaction between Triptophan and Histidine", Department of Chemistry (completed). Following position: graduate school in UWO, research group of M. Kartunnen.
13. Sept. 2020-April 2021: "Study of Cholera Toxin Assembly Mechanism by Molecular Dynamics", Department of Biochemistry, Following position: graduate school in UWO.
14. Sept. 2019-April 2020: "Effect of Explicit and Implicit Solvents in the Binding Free Energies of Protein Complexes", Department of Chemistry (completed). Present position: graduate school in UWO - research group of J. Noel.
15. Sept. 2019-April 2020: "Computational modelling of water clusters relevant to the molecular mechanism of thunderclouds" Department of Chemistry (completed) **Awards received while in my lab:** Outstanding Oral Presentation Award in Physical, Theoretical, & Computational Chemistry, SOUSCC, Ryerson University, Toronto. Following position: Regulatory Scientist in Estee Lauder for 2 years and presently, Account Manager with Fisher Scientific, Western Research Park, London, Ontario.
16. Sept. 2019-April 2020: "Exploration of the Effects of Confinement on the Structure and Binding Energy of Protein Complexes with Molecular Dynamics", Department of Chemistry (completed). Following position: Continuing studies in the Department of Computer Science, Western.
17. Sept. 2019-April 2020: "The Implementation of Machine Learning to Predict the Solubility of Simple Organic Molecules" Department of Chemistry (completed). Following position: Medical school, University of Saskatchewan. **Awards received while in my lab:** Alumni Gold Medal, Department of Chemistry, UWO.
18. Sept. 2019-April 2020: "A computational characterization of the distribution of multi-valent ions within highly charged aerosol droplets", Department of Chemistry (completed)
19. Sept. 2019-April 2020: "Modelling of proton transfer reactions in a bulk solution of acetonitrile molecules using path integral method", Department of Chemistry (completed). Following position: apply to the

graduate school.

20. Sept. 2019-April 2020: Fourth year student from the Department of Computer Science, UWO (completed). Following position: apply to the graduate school.
21. Sept. 2018-April 2019: Computer Science Department, UWO. **Title of the thesis:** Protein interaction networks. (*completed*)
22. Sept. 2018-April 2019: Biochemistry Department, UWO. **Title of the thesis:** Effect of ions in the stability of protein complexes. (*completed*) **Following position:** Graduate student in the Biochemistry Department, UWO and then student at the school of Medicine, Australia.
23. Sept. 2017-April 2018: **Title of the thesis**: Interplay between hydrophilic/hydrophobic interactions in droplets." (*completed*) Following position: On June 15, 2023 the student defended successfully their PhD thesis in computational chemistry in Pennsylvania State University. Ryan has received a position at the Computational Research Center directed by Prof. Roberto Car, at Princeton University.
24. Sept. 2016-April 2017: **Title of the thesis**: "Do star formations of droplets establish a growth pattern for snowflakes?" (*completed*) **Distinctions received while in my lab** Role model student in the year (Departmental). (following position: Private sector).
25. Sept. 2016-April 2017: **Title of the thesis**: "Modelling of the interactions of proteins in vapour-liquid interface" (*completed*) (following position: grad student in the group of Prof. M. Kartunnen).
26. Sept. 2015-April 2016: **Title of the thesis**: Characterization of the "star" morphologies of charged droplets" (*completed*)
27. Sept. 2014-April 2015: **Title of the thesis**: "Treatment of Electrostatic Interactions in Molecular Simulations" (*completed*) (following position: student in the School of Optometry and Vision Science, University of Waterloo).
28. Sept. 2013-April 2014: **Title of the thesis**: "Monte Carlo Modelling of Charged Nanodroplets" (*completed*).
29. Sept. 2013-April 2014: **Title of the thesis**: "Effect of charge distribution on the stability of droplets" **Awards received while in my lab** (i) *2nd Prize* for his presentation on the thesis project in the SOUSCC conference, Analytical Chemistry Session, March 29, 2014, University of Windsor and (ii) Hypercube Scholar Award, UWO); (*completed*). (following position: Consulting Analyst in the Info-Tech Research Group)
30. Sept. 2013-April 2014: **Title of the thesis**: "Interactions of complexes of macromolecules in charged nanodroplets" **Awards received while in my lab:** (i) *1st Prize* in the SOUSCC conference, Physical Chemistry Session, March 29, 2014, University of Windsor, (ii) received the Ontario Graduate Scholarship but declined, (iii) Western Gold Medal for Honours Specialisation in Chemical Biology); (*completed*). (following position: Medical School, McMaster University; completed her medical studies and also her specialization in pediatrics)
31. Sept. 2012-April 2013: **Title of the thesis**: "Charge-Induced Instability in Droplets with Charged Macromolecular Complexes – Study of siRNA in Aqueous Droplets" *(completed)* (oral presentation in the SOUSCC conference, McMaster University, March 30, 2013, Chemical Physics Symposium in Waterloo, November 2013) (following position: grad student, Chemistry, UWO)
32. Sept. 2011-April 2012: **Title of the thesis**: "Computational modeling of the Solvation and Diffusion of Doxorubicin and Fluorouracil in Water" *(completed)* (following position that time: medical school UWO)
33. Sept. 2010-April 2011: **Title of the thesis**: "Analysis of the structure of PEG-$(Na^+)_n$ in a water droplet by molecular dynamics". *(completed)*
34. Sept. 2008-April 2009: **Title of the thesis**: "Molecular dynamics methods for simple Lennard-Jones systems and applications in diffusion in zeolites". *(completed)* (following position: medical school UWO)
35. Sept. 2004-April 2005: **Title of the thesis**: "Sampling of reactive paths for computations of reaction rates in the condensed phase. Applications in reactions in clusters.". *(completed)*

36. Sept. 2003-2005: **Title of the thesis**: "Equilibrium and dynamic properties of peptides in solution". *(completed)*
37. Sept. 2003-April 2004: (Dept. of Biochemistry and Applied Mathematics), **Title of the thesis**: "Molecular Dynamics study of alanine dipeptide in aqueous neutral and charged droplets". *(completed)* (following position : graduate of Pharmacy school, Alberta) (Minh received a number of prestigious awards while she was in my lab)
38. Sept. 2003-April 2004: **Title of the thesis**: "Testing of Sampling methods for reactive paths for computations of reaction rates in solution". *(completed)* (following position: graduate of Dental school, UWO)
39. Sept. 2003-April 2004: **Title of the thesis**: "Properties of $(NH_3)(H_2O)_n (n = 1 - 4)$ clusters on a carbon nanotube and confinement effects on the structure of a fluid" *(completed)*
40. May 2002-August 2002: 4th year undergraduate student. **Title of the thesis**: "Fragmentation processes of charged droplets." *(completed)* (Employed by pharmaceutical industry)
41. Sept. 2001-April 2002: **Title of the thesis**: "Efficient Monte Carlo schemes for computer simulations of polymer systems." *(completed)*
42. Sep. 1999- April 2000: **Title of the thesis**: "Diffusion dynamics in liquid clusters." **Awards received while in my lab:** *First prize in Physical Chemistry* in the Southwestern Ontario Undergraduate Student Chemistry Conference (SOUSCC). Hunter presented their research as a poster presentation in the *Canadian Computational Chemistry Conference*, Quebec, 2000. *(completed)* (following position: graduate of Computer Engineering school and employed in the industry)

Graduate Students - Principal Supervisor: S. Consta

1. Sept. 2023- Dec. 2027: MSc Student Thesis title "Modelling of Chemistry and of Conformations of Peptides in droplets". Number of awards while in my lab: 2
2. Sept. 2017-May 2022: PhD Student Thesis title "Computational Modelling of Interfacial Properties of Droplets". Number of awards while in my lab: 3.
3. May 2013-December 2018: PhD Student Thesis title "Computational Studies on Nucleic Acid-Ion Interactions in Droplets and Bulk Solution". Number of awards while in my lab: 2.
4. May 2013-April 2018: PhD Student Thesis title "Computational and Analytical Modelling of Droplet-Macorion Interactions". Number of awards while in my lab: 11.
5. September 2010-2014: PhD student (co-supervised) **Title of the thesis**: "Mechanisms of Release of Anti-Cancer Drugs in the Cell Environment"
6. September 2008-Sept. 2010: MSc Student (co-supervised) **Title of the thesis**: "Experiments and Molecular Simulations of Oiling-out Phenomenon"
7. May 2002-December 2006 : MSc Student **Title of the thesis**: "Fragmentation mechanisms of charged binary clusters."
8. Sept. 2002-Oct. 2005 : MSc Student **Title of the thesis**: "Nucleation mechanisms and cluster size distributions in vapour of mixture of methanol-ethanol."
9. Sept. 2001-Aug. 2003: MSc Student, **Title of the thesis**: "Crystallization of NaCl in aqueous environment" Number of awards while in my lab: 1.

Postdoctoral Fellows - Principal Supervisor: S. Consta

PDF supervision: 10