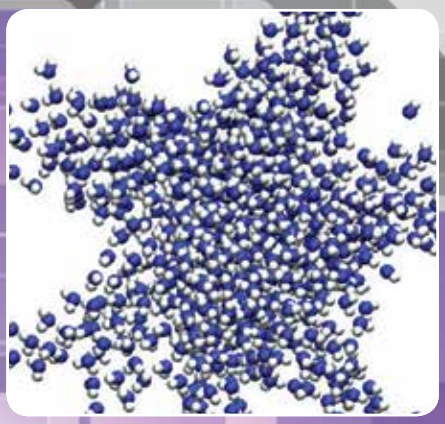
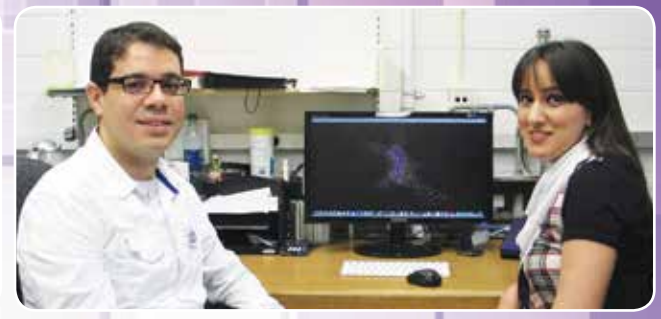
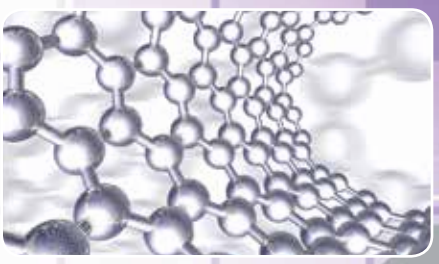
GRADUATE STUDIES | Department of Chemistry

Theory and Computation







Western Science

WESTERN SCIENCE

Department of Chemistry

The Department of Chemistry at Western University offers a large and vibrant, research-intensive environment for more than 100 graduate students.

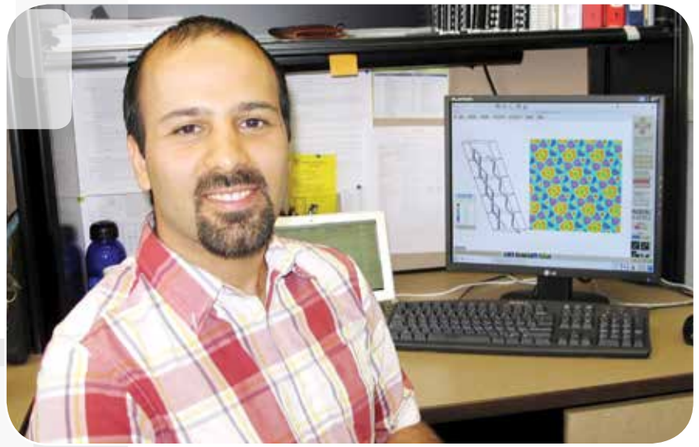
Taking a modern view of the chemical sciences, the four main research themes reflect Western's open-minded and multidisciplinary approach to research. These themes include: Chemical Biology and Biomaterials; Synthesis, Catalysis and Molecular Materials; Materials: Design, Function and Characterization; and Theory and Computation.

We are proud to boast over 25 NSERC-funded researchers, some of whom are Tier I and II Canada Research Chairs and Industrial Research Chairs with numerous links to academic and industrial partners, and some of the finest research facilities in Canada.

Our researchers play leading roles in organizations within Western, including: The Centre for Advanced Materials and Biomaterials Research (CAMBR), Surface Science Western, and the Western Nanofabrication Facility, and publish regularly in top tier peer-reviewed journals. Graduate students can expect their results to be disseminated globally. They may also receive opportunities to conduct applied research in collaboration with industrial partners.

Theory and Computation

The "Theory and Computation" research theme at Western is comprised of the research groups of Prof. Styliani Constas and Prof. Viktor Staroverov. The Constas Group conducts computational condensed-phase research in order to understand the dynamics of chemical reactions in solution, proton transfer reactions, conformational changes of macromolecules, and disintegration mechanisms of charged nanodroplets. The Staroverov Group develops density-functional methods and computer codes for predicting physical and chemical properties of matter. Using these methods they elucidate mechanisms of chemical reactions and unravel the intricacies of chemical bonding in molecules and solids.



Academic Snapshot

30
full-time faculty

100+
full-time graduate students

Over 7,500
students taught annually

2,500th BSc
by 2014

200th PhD
by 1986

475th PhD
by 2014

A Tradition of Research

Average annual research revenue
$4,000,000

FIRST
publication in 1915

100
publications by 1962

1,000
publications by 1975

2,000
publications by 1985

6,000
publications by 2012

The Constas Computational and Theoretical Physical Chemistry Group

Styliani Constas, Associate Professor

PRIMARY RESEARCH FOCUS
The Constas Group employs theory and computer simulation methods to investigate the physical chemistry of macromolecule-ion and solvent interactions in bulk solution and charged droplets. The computational methods are based on the use of advanced Molecular Dynamics and Monte Carlo techniques. Practical applications are in natural aerosols, electrospray ionization techniques, and biological systems.

INDUSTRIAL, ACADEMIC AND OTHER COLLABORATORS
The Constas Group collaborates with both industry and academic partners, in particular AB-SCIEX and the Department of Chemistry at the University of Cambridge in the United Kingdom.

RECENT PUBLICATION
S. Constas*, A. Malevanets "Manifestations of Charge Induced Instability in Droplets Effected by Charged Macromolecules'' *Phys. Rev. Lett.* **2012**, *109*, 148301.

"Being a part of the Constas lab has been an excellent learning experience. The challenging and exciting research environment has prepared me with a diverse skill set and has been a wonderful opportunity."

– Falana Sheriff, PhD

FOR MORE INFORAMATION
www.theory.chem.uwo.ca
or contact sconstas@uwo.ca

The Staroverov Quantum Chemistry Group

Viktor Staroverov, Associate Professor

PRIMARY RESEARCH FOCUS
The Staroverov Group develops theoretical methods and computer programs for studying electronic structure, physical properties, and chemical reactions of molecules and solids. The focus of our research is on the Kohn-Sham density-functional method, particularly on designing new exchange-correlation approximations and model effective potentials. We also use computational chemistry methods to solve practical problems of chemistry and spectroscopy.

RECENT PUBLICATIONS
I. G. Ryabinkin, A. A. Kananenka, and V. N. Staroverov* "Accurate and Efficient Approximation to the Optimized Effective Potential for Exchange" *Phys. Rev. Lett.* **2013**, *111*, 013001.

A. P. Gaiduk, D. S. Firaha, and V. N. Staroverov* "Improved Electronic Excitation Energies from Shape-corrected Semilocal Kohn-Sham Potentials" *Phys. Rev. Lett.* **2012**, *108*, 253005.

"Research in our group is organized in a very efficient manner. My independence is strongly encouraged and I have the freedom to stick to my work habits. At the same time I can get help whenever I need it because my supervisor is available for discussions at any time. I also receive a lot of valuable career advice and tips on resumé preparation and scholarship applications."

– Alex Gaiduk, PhD

ACCOMPLISHMENTS AND PAST GRADUATES
Students associated with the Staroverov Group are recipients of major awards including:

- Alex Gaiduk, PhD 2013, Paul De Mayo Award for Excellence in Chemical Research
- Sviataslau Kohut, PhD student, Ontario Trillium Scholarship
- Pavel Elkind, MSc, 2009, Marie Curie Research Fellow

FOR MORE INFORMATION
http://publish.uwo.ca/~vstarove
or contact vstarove@uwo.ca

Western Science

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www.facebook.com/ChemistryatWestern