Chemistry

Graduate Studies at Western

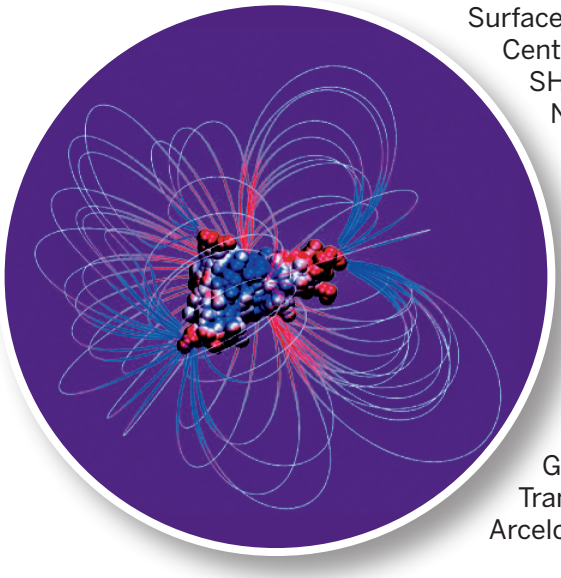
Energy and Mechanism

The Energy and Mechanism theme affiliates researchers whose interests include chemical kinetics and transport phenomena in chemical, electrochemical, metallurgical, and radiation-induced reactions; environmental studies relevant to industrial processes and nuclear power generation; computer simulations in condensed phase, computational chemistry, and electronic structure theory.

The goal of the kinetics and transport studies (Profs. Clara Wren and David Shoesmith) is to solve various industrial corrosion and environmental contamination problems such as chemical behaviour of nuclear reactor fuel, containment of high-level radioactive waste, and contaminant transport in ground waters. This involves the use of a wide range of electrochemical techniques adapted to aggressive conditions and various surface and near-surface analytical methods such as X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy, scanning electron microscopy (SEM), and neutron reflectometry.

The objectives of the computational condensed-phase research (Prof. Styliani Constas) is to understand the dynamics of activated processes such as chemical reactions in solution, proton transfer reactions, conformational changes of macromolecules and disintegration mechanisms of charged nanodroplets. These studies involve computer simulations using molecular dynamics and Monte Carlo techniques. Students in the quantum chemistry group of Prof. Viktor Staroverov develop 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.

Our research facilities and industrial partners include:



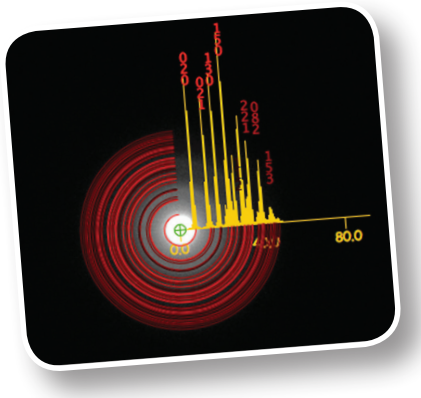
Surface Science Western - www.surfacesciencewestern.com
Centre for Advanced Materials and Biomaterials Research - www.uwo.ca/cambr
SHARCNET - www.sharcnet.ca
Nanofabrication Facility - www.uwo.ca/fab/
Ontario Power Generation - www.opg.com
Bruce Power - www.brucepower.com
Ministry of Transport Ontario - www.mto.gov.on.ca
Nuclear Waste Management Organization - www.nwmo.ca
Atomic Energy of Canada Limited - www.aecl.ca
Acsion Industries - www.acsion.com
Canadian Institute for Neutron Scattering - www.cins.ca
Natural Resources Canada - www.nrcan.gc.ca
Argonne National Laboratories - www.anl.gov
Swedish Nuclear Fuel Company - www.skb.se
General Motors Canada - www.gm.ca
Trans Canada Pipelines - www.transcanada.com
Arcelcor Mittal - www.dofasco.ca

Our recent MSc and PhD graduates have successfully found positions in academia (Los Alamos Labs, University of Strathclyde, University of California, Western) and industry (Kinectrics, Cameco, Atomic Energy of Canada, CANDU Energy Incorporated, Nova Research and Technology, CANMET, Blade Energy, RCMP Forensic, and other companies)

"My research at Western involves investigation of the chemical composition and phase structure of metal oxide films", says Quintin Knapp, a PhD candidate in the Clara Wren group." In our lab we simulate the high temperature and radiolytic environments experienced by materials within nuclear reactors. We investigate film properties under these conditions using a range of electrochemical and surface sensitive techniques such as impedance spectroscopy and scanning electron microscopy. The resulting information is used by the nuclear industry as it tells us about the kinetics of steel corrosion and the lifetime of reactor materials. Working at Western has allowed me to pursue my passion using cutting-edge technology and allowing me to work with some of the most influential people in my field."

Western Science

Quick facts about the Chemistry Department



Academic History

Founded 1882

Over 3000 Students Taught Annually
100 plus Students Graduating Annually

2000th BSc by 1990
200th PhD by 1986
300th PhD by 1998

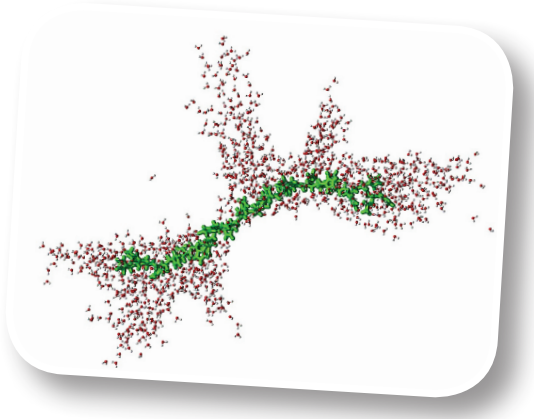
30 Full-Time Faculty
110 Full-Time Students Enrolled

A Tradition of Research

Average Annual Research Revenue
$4,000,000

First publication in 1915
100 publications by 1962
1000 publications by 1975
2000 publications by 1985
4000 publications by 2000

Faculty Members in the Energy and Mechanism Theme



Conformational changes of a polyhistidine (green coloured) in a cluster of water molecules (red-white colours) and analysis of the electrostatic field on the surface of the polyhistidine-water cluster.

Stella Constas

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Research in our group focuses on the development of computational methods that capture the momentary fluctuations in the molecules of solvents and solutes in solutions or solids that lead to chemical and physical phenomena. These methods allow us to study the mechanism and rates of chemical reactions such as acidic-basic properties of aminoacids, conformational changes of peptides and phase transformations of materials such as titanium oxide nanotubes. The motions of the molecules are simulated with Monte Carlo and Molecular Dynamics methods adopted for capturing the molecular fluctuations. The outcomes of our studies explain mechanisms and show ways to control various chemical processes.

David Shoesmith

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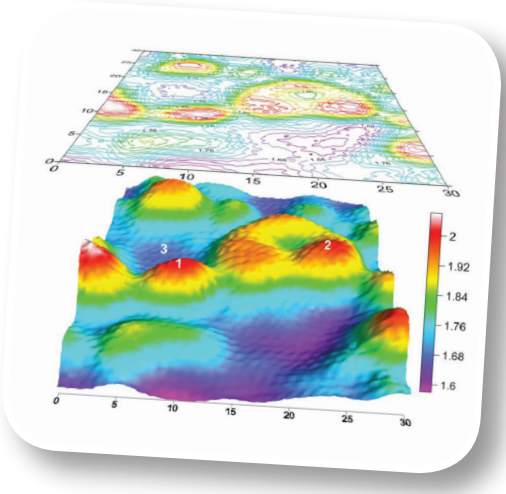
Our research involves the electrochemistry, analytical science and corrosion of materials. We study the kinetics of surface reactions, and reactions on surfaces in aqueous solutions and analyze the chemical and physical properties of the surfaces they occur on. We use a wide range of electrochemical techniques supplemented by both in-situ and ex-situ surface analytical and spectroscopic methods, including focused ion beam milling, X-ray photoelectron spectroscopy and Raman spectroscopy. Our primary goal is to solve industrial materials problems and we are funded by companies in the energy (nuclear, oil and gas) and manufacturing (automobile) industries.



Electrochemical surface reactivity map recorded by a scanning electrochemical microscopy for uranium dioxide showing the variations in reactivity with degree of oxide non-stoichiometry

Western Science

Viktor Staroverov
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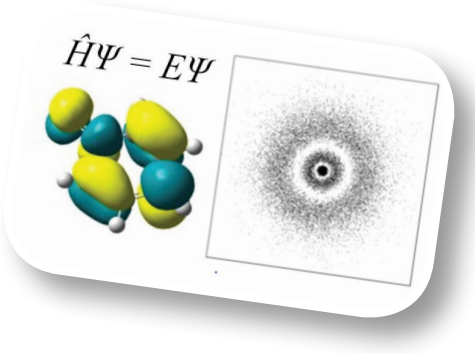
We develop computational methods for studying the electronic structure, physical properties, and chemical reactions of molecules and solids. The focus of our research is on the Kohn-Sham density-functional method, particularly on designing new density-functional approximations in the form of model Kohn-Sham potentials. Another theme is development of new techniques for solving the Schrödinger equation for systems of confined electrons. We also use computational chemistry methods to solve practical problems of chemistry and spectroscopy. Applied computational research in our group centers on elucidating the mechanisms of chemical reactions, understanding the electronic structure of electrides, and unraveling the intricacies of chemical bonding in chemical compounds under high pressure.



Clara Wren
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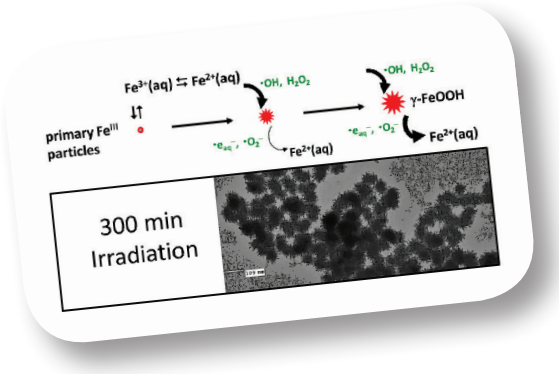

Wren's research areas are in Radiation Chemistry and Materials Performance, with particular focuses on the applications to colloid formation, bi-phasic separation and corrosion research. Since water radiolysis produces both highly oxidizing (e.g., •OH) and highly reducing (e.g., $\bullet e_{aq}^-$, $\bullet O_2^-$) species simultaneously, it can induce unusual aqueous redox chemistry. This chemistry can drive reactions involving water-solid and water-liquid interfacial mass and charge transfer, such as colloid (or nanoparticle) formation and corrosion. To understand radiation-induced interfacial processes, the Wren research group has carried out studies on: (1) the impact of pH/redox-controlling agents on the water radiolysis chemistry, (2) formation of metal oxide colloids from dissolved metal ions, (3) corrosion of steel, and (4) micelle formation and biphasic mixing in water-ionic liquid systems. A range of chemical, electrochemical and surface analytical techniques, in combination with model calculations, are used.

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