UNIVERSITY OF WATERLOO

AI FOR SCIENCE & ENGINEERING WORKSHOP

JAN. 18th - JAN. 20th, 2022
(3 half-days)
LIVE EVENT via MS Teams

WATERLOO.AI
WATERLOO ARTIFICIAL INTELLIGENCE INSTITUTE

WATERLOO INSTITUTE FOR nanotechnology

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WATERLOO ARTIFICIAL INTELLIGENCE INSTITUTE

Waterloo Artificial Intelligence Institute

The Waterloo Artificial Intelligence Institute (Waterloo.AI) is dedicated to fostering and promoting research in all aspects of artificial intelligence (AI) and machine learning (ML). Waterloo.AI consists of over 200 professors and their research associates, spanning all six of the faculties at the University of Waterloo and more than 35 departments and schools. Our researchers tackle many of the most challenging problems in foundational and applied AI and ML, including its social, ethical, and policy implications.

Waterloo.AI was launched officially in early 2018 with generous support from the Faculty of Engineering (the largest faculty of engineering in the country), the Faculty of Mathematics (which houses the largest Computer Science department in the country), the Office of the Vice-President Academic & Provost, and the private industry. The founding co-directors of the Institute are Professor Fakhri Karray (Electrical and Computer Engineering, Faculty of Engineering) and Professor Peter van Beek (Computer Science, Faculty of Mathematics).

WATERLOO INSTITUTE FOR nanotechnology

Waterloo Institute for Nanotechnology

The Waterloo Institute for Nanotechnology (WIN) is Canada's largest nanotechnology institute, and an innovation powerhouse in the four key theme nanotechnology research areas of smart and functional materials, connected devices, next generation energy systems and, therapeutics and theranostics.

Housed in the custom-built Mike and Ophelia Lazaridis Quantum-Nano Centre (QNC), WIN scientists and engineers have access to state-of-art research infrastructure to support their endeavours. Aligning their research interests with the United Nations Sustainable Development Goals, WIN members are creating new materials and systems to improve the economy, the environment, our health and welfare, and society as a whole.

Workshop Agenda
Day 1 Schedule – Tuesday 18th January 2022

* all times in Eastern Standard Time unless otherwise noted

Moderator for Day 1: Harold Godwin, Managing Director, Waterloo.AI

TIME	SCHEDULE
8:40 – 8:45am	Harold Goldwin , Managing Director at Waterloo.AI: Welcome and Territorial Acknowledgment
8:45 – 8:50am	Bessma Momani, Associate Vice-President of Interdisciplinary Research
8:50 – 8:55am	Laurent Servant, Vice-President, International Networks, University of Bordeaux France
8:55am – 9:00am	Mary Wells, Dean of Engineering, University of Waterloo
9:00 – 9:45am	**Keynote Speaker 1**: Jill Becker, CEO, Kebotix Inc:" Transforming Materials Discovery: Today"
	Technical Talk Session 1: AI for Security and Public Health Monitoring
9:45am – 10:05am / 15h45 – 16h05 CET	Jenny Benois-Pineau, University of Bordeaux: "Monitoring of Frail Subjects for Risk Situation Detection with AI Tools"
10:05 – 10:25am /16h05 –16h25 CET	Patricia Nieva (MME) with William Melek (MME): "ML models for distance optimization for infectious disease-tracing (including Covid-19) using Bluetooth enabled devices"
10:25 – 10:45am /9:25 – 9:45am CST	Gayo Diallo, University of Bordeaux: "Data and Knowledge Integration for Digital Public Health"
	Technical Talk Session 2: AI for New Materials Discovery
10:45 – 11:05am	Peyton Shi (ECE): "AI – a potentially powerful tool for nano-material characterization"
11:05 – 11:25am	Rodney Smith (Chem): "Empowering Spectroscopic Analysis Using the Interpretive Capabilities of ML"
11:25 – 11:45am	Scott Hopkins (Chem): "ML molecular properties from mass spectrometry data"
11:45 – 12:20pm	***Break***
12:20 – 12:40pm /18h20 – 18h40 CET	Stéphane Gorsse, University of Bordeaux: "Machine Learning Assisted Design and Development of High-entropy Alloys"
12:40 – 1:00pm /18h40 – 19hr00 CET	Mario Maglione, University of Bordeaux: "DIADEM Project: Towards AI in Materials Science"

Day 2 Schedule – Wednesday January 19, 2021

*all times in Eastern Standard Time unless otherwise noted

Moderator for Day 2: Oleg Stukalov, Business Development Manager, Waterloo Institute for Nanotechnology

TIME	SCHEDULE
8:55-9:00am	Terry McMahon, Professor, Department of Chemistry: Day 2 Opening Comments
9:00 – 9:45am /15h00 – 15h45 CET:	**Keynote Speaker 2**: Laurent Simon, University of Bordeaux: "AI and the University of Bordeaux: Opportunities and Challenges"
	Technical Talks Session 3: AI for Medical Applications and Diagnoses
9:45 – 10:05am	Mohammad Kohandel (AM): "AI for biomedical data"
10:05 – 10:25am	Melanie Campbell (PAS): "Using AI to enable the eye as a window on neurodegenerative diseases of the brain"
10:25 – 10:45am	Juewen Liu (Chem): "Test tube evolution of DNA aptamers as biosensors"
10:45 – 11:00am	***Break***
	Technical Talks Session 4: AI for Water Quality and Environment
11:00 – 11:20am	Frank Zhu (CEE): "PlasticNet – Deep learning for automatic microplastic recognition in water via FT-IR Spectroscopy"
11:20 – 11:40am	Vassili Karanassios (Chem): "Applications of Artificial Intelligence (and related topics) in Micro and Nano for Water and Health"
11:40 – 12:00pm	Sushanta Mitra (MME): "Predictive capability of water quality monitoring sensors: Need for machine learning"
	End of Day 2

Day 3 Schedule –Thursday January 20, 2022

* all times in Eastern Standard Time unless otherwise noted

Moderator for Day 3: Lisa Pokrajac, Assistant Director, Waterloo Institute for Nanotechnology

TIME	SCHEDULE
10:00-10:05am	Mark Giesbrecht, Dean of Mathematics: Day 3 Opening Comments
10:05 – 10:45am /16h05 – 16h45 CET	**Keynote Speaker 3**: Wilfred van der Wiel, NanoElectronics Group, Director BRAINS Centre for Brain-Inspired Nano Systems, University of Twente, Netherlands: "Material Learning"
	Technical Talks Session 5: AI for Improved Manufacturing and Industry Applications
10:45 – 11:05am	Kaan Erkorkmaz (MME): "Boosting Manufacturing through Virtualization and Intelligence"
11:05 – 11:25am	Michel Fich (PAS): "ML tools for predicting maintenance requirements on a distant remote-controlled facility"
11:25 – 11:45am	Qinqin Zhu (ChE): "Dynamic Latent Variable Analytics for Inferential Sensor Modeling and Supervised Monitoring"
11:45 – 12:05pm	Laurent Simon, University of Bordeaux: "AI for Critical Systems: Progresses and Limits"
12:05 – 1:00pm	***Break***
	Technical Talks Session 6: Foundational AI
1:00 – 1:20pm	Vijay Ganesh (ECE): "Logic Guided Machine Learning"
1:20 – 1:40pm	George Shaker (ECE): "AI-powered Radar Sensing"
1:40 – 2:00pm	Roger Melko (PAS): "Generative models and quantum computers"
2:00 – 2:20pm	Yimin Wu (MME): "Brain Inspired Computing for Artificial Intelligence"
2:20 – 2:40pm	Sylvain Saïghi, University of Bordeaux: "Towards an Energy Sustainable AI"
2:40 – 3:00pm	**Closing remarks and next steps**: Sushanta Mitra (WIN) and Vijay Ganesh (Waterloo.Ai)
	End of workshop

List of abbreviations for UW Departmental Affiliations:
AM: Applied Mathematics
CEE: Civil & Environmental Engineering
ChE: Chemical Engineering
Chem: Chemistry
ECE: Electrical & Computer Engineering
MME: Mechanical & Mechatronics Engineering
PAS: Physics & Astronomy

Keynote Speaker 1

Jill S. Becker
CEO and Founder
Kebotix Inc.
Cambridge, Massachusetts

Title: Transforming Materials Discovery: Today

Biography: Dr. Jill S. Becker is CEO of Kebotix, a technology platform that is reinventing the materials industry and enables a new age of discovery of new materials using AI, machine learning, and robotics. Dr. Becker received her undergraduate degree from the University of Toronto, followed by Masters and Ph.D. studies in chemistry from Harvard University. Her Ph.D. thesis research led to the creation of Cambridge NanoTech Inc., which was subsequently acquired by Veeco. Dr. Becker is also involved in strategic consulting, venture capital, and entrepreneurship support at Harvard. She is a past Ernst and Young Entrepreneur of the Year winner in energy & materials and a member of YPO. In her spare time, she loves to travel and spend time with her friends & family. Like most chemists, Jill is a foodie and deeply appreciates haute gastronomy.

Abstract: Kebotix has developed the world's first AI- and robotics-driven closed-loop platform that autonomously discovers, synthesizes, identifies and "dreams up" new advanced materials and chemicals. This breakthrough ushers in a new age of high-speed innovation and shifts the entire paradigm of how science advances. We are at the technological frontier, pushing the boundaries of science.

New advanced materials with superior performance characteristics are required to solve the world's most pressing problems in clean energy, agriculture, etc.Currently, our technology is helping large chemical and materials companies embrace the digital revolution for creative design of new materials and chemicals as a way of shifting from a cost-cutting strategy toward simultaneous improvement of short-term performance and realization of long-term financial growth. Our technology helps these companies in multiple ways. One is to capitalize on new opportunities by strengthening and accelerating their innovation efforts. Another is to realize profit by revamping their offerings and developing differentiated, market-oriented chemical products. Our technology offers customers the opportunity to do more with less, thus lowering the cost of running a business.Over the next few years, our technology will continue to be a catalyst in the development of environmentally friendly chemicals and for the design of chemical processes that lessen consumption of energy and generation of waste. Taking the serendipity out of science and bringing R&D to scale is at the heart of Kebotix's AI technology platform.

Speaking of heart, Kebotix has a big one for our planet and people. Our mission, in fact, is to champion sustainability, improve public health and eliminate the production of hazardous substances by developing transformative technologies that facilitate important first steps toward tackling some of the world's biggest challenges of the 21st century.We will discuss Kebotix's innovative and transformative technology, and show how it harnesses the immense potential of AI by sharing several compelling and topical use cases.

Keynote Speaker 2

Laurent Simon
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University of Bordeaux
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Title: AI and the University of Bordeaux: Opportunities and Challenges

Abstract: Artificial intelligence is strongly present in Bordeaux. In the context of the meeting organized with Waterloo, we will present the most salient projects that are currently developed on the site. This presentation is not intended to be exhaustive but rather to stimulate discussions around a (necessarily partial) selection of what is currently being done around AI in Bordeaux.

Biography: Professor in Computer Science at the engineering school Bordeaux INP and at the LaBRI. His main research interest is around propositional logic and the design of efficient algorithms for solving real world problems represented under this formalism (typically Constraints and SAT). He is also working on the more general frameworks Knowledge Representation and Compilation.

Keynote Speaker 3

Wilfred van der Wiel

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Title: Material Learning

Abstract: The strong increase in digital computing power in combination with the availability of large amounts of data has led to a revolution in machine learning. Computers now exhibit superhuman performance in activities such as pattern recognition and board games. However, the implementation of machine learning in digital computers is intrinsically wasteful, with energy consumption becoming prohibitively high for many applications. For that reason, people have started looking at natural information processing systems, in particular the brain, that operate much more efficiently. Whereas the brain utilizes wet, soft tissue for information processing, one could in principle exploit any material and its physical properties to solve a problem. Here we give examples of how nanomaterial networks can be trained using the principle of *material learning* to take full advantage of the computational power of matter.

We have shown that a designless network of gold nanoparticles can be configured into Boolean logic gates using artificial evolution. We further demonstrated that this principle is generic and can be transferred to other material systems. By exploiting the nonlinearity of a nanoscale network of boron dopants in silicon, we can significantly facilitate classification. Using a convolutional neural network approach, it becomes possible to use our device for handwritten digit recognition. An alternative material learning is approach is followed by first mapping our Si:B network on a deep neural network model, which allows for applying standard machine learning techniques in finding functionality. Finally, we show that the widely applied machine learning technique of gradient descent can be directly applied *in materio*, opening up the pathway for autonomously learning hardware systems.

Biography: Wilfred G. van der Wiel is full professor of Nanoelectronics and director of the BRAINS Center for Brain-Inspired Nano Systems at the University of Twente, The Netherlands. He holds a second professorship at the Institute of Physics of the Westfälische Wilhelms Universität Münster, Germany. His research focuses on unconventional electronics for efficient information processing. Van der Wiel is a pioneer in Material Learning at the nanoscale, realizing computational functionality and artificial intelligence in designless nanomaterial substrates through principles analogous to Machine Learning. He is author of 125 journal articles receiving over 7,500 citations.

Speaker Profiles

Jenny Benois-Pineau
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Title: Monitoring of Frail Subjects for Risk Situation Detection with AI Tools

Abstract: Development and application of AI tools by (supervised) Deep Learning approach for healthcare domain rises new challenges as it requires complex architectures processing multimodal, heterogeneous, noisy and imbalanced temporal data. Such is the problem of monitoring of fragile subjects in an ecological environment for risk situation detection.

The definition of the target taxonomy is a multidisciplinary task which has been conducted by BPH – UB and Department of Kinesiology-UW. Data collection scenarios on fragile subjects had also to be developed and adapted. Data collection in a wearable IoT setting requires an adequate application on a commun mobile phone (androïde) platform which was developed by INFLEXYS company a Hight-Tech SME from Aquitainia region.

Acceptability of such kind of IoT devices required an iterative adjustment for better acceptability for users and also the respect of data usage regulations with a total anonymization.

A novel Deep Learning Hybrid architecture has been developed as a twin hybrid DNN with a branch processing sensors signals including physiological and motion sensor data and a contextual wearable video sensor. The combination of an GRU (for signals) and of a 3D Convolutional network ResNet (for video data) with a commun self-attention block allows attaining 83% accuracies on a subset of risk situations from designed taxonomy. For data ingestion, data pre-processing with synchronization, imputation and balancing algorithms have been developed. At present, a new hybrid transformer architecture is being developed with the possibility of explanation of decisions on the data. This will ensure trustworthy into proposed AI tools for risk situation detection.

Biography: Jenny Benois-Pineau is a professor of Computer Science at the University Bordeaux. Her topics of interest include image/multimedia, artificial intelligence in multimedia and healthcare. She is the author and co-author of more than 230 papers in international journals, conference proceedings, books and book chapters. She has tutored and co-tutored 27 PhD students She is associated editor of SPIC, ACM MTAP, senior associated editor JEI SPIE journals. She has served in numerous program committees in international conferences: ACM MM, ICMR, CIVR, CBMI, IPTA, MMM, and organized WS at the major conference as ACM MM, IEEE ICIP, ICPR … She has been coordinator or leading researcher in EU – funded and French national research projects and projects with French companies. She was invited for lecturing as a distinguished researcher at the Universities of Madrid, (Spain), Klagenfurt (Austria), Ben Gurion (Israel), NJIT (USA), UAM, CITEDI (Mexico) and gave invited lectures at the UNC at Chapel Hill, Carnegie Melon, Brooklynn Polytechnic (USA), University of Sussex (GB) and UCL (Belgium). She is a member of IEEE TC IVMSP. She has Knight of Academic Palms grade.

Melanie Campbell

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Title: Using AI to enable the eye as a window on neurodegenerative diseases of the brain

Abstract: In this talk Prof. Melanie Campbell will discuss her novel, patented method and the application of machine learning methods to images of protein deposits in the retina of the eye as biomarkers of neurodegenerative diseases in the eye and brain. During embryonic development, the eye develops as an extension of the brain and contains neural cells, similar to those in the brain. Campbell's group was one of the first to show that deposits of the protein amyloid beta, a key diagnostic of Alzheimer's disease (AD) are found in the retina in association with neural cells. Campbell then developed and patented a novel, dye-free method for imaging the deposits with polarised light. The method can identify presumed amyloid deposits with 100% sensitivity in retinas of those with a diagnosis of AD. In addition, the number of amyloid deposits predicts the severity of amyloid beta pathology in the brain and the overall severity of Alzheimer's disease pathology. Amyloid beta expresses in the eye and brain 15-20 years before the onset of disease symptoms. Early, inexpensive detection in the retina would allow lifestyle changes which slow the disease and the development of earlier treatments. In collaboration with her research students, Campbell has shown (and patented) that machine learning methods can predict which polarimetric signals in her dye-free method of imaging retinal deposits predicted that they would show a positive response to an amyloid dye. Machine learning approaches also allowed us to differentiate images of deposits of alpha synuclein, a biomarker of Parkinson's disease from images of amyloid beta, associated with AD. Furthermore, machine learning can assist in the differentiation of images of amyloid beta in the anterior neural retinal layers, associated with AD from deposits in the posterior retina (presumed to be associated with age related macular degeneration, a neurodegenerative eye disease). These approaches hold great promise as an earlier, less invasive, readily available differential diagnostic which will enable less expensive testing of promising treatments and earlier, more accurate diagnosis of neurodegenerative conditions of the eye and brain.

Biography: Melanie Campbell earned a BSc from the University of Toronto, an MSc from the University of Waterloo and, from the Australian National University, a PhD in Applied Mathematics and Physiology. Following a CSIRO Fellowship at the Institute of Mathematics and Statistics in Canberra, Campbell returned to Canada with an NSERC University Research Fellowship.Prof. Campbell collaborated in the first real-time images of cone photoreceptors in the eye, using adaptive optics and she uses polarization imaging to make invisible structures visible. Imaging applications include a biomarker of Alzheimer's disease, using the retina as a window on the brain. She undertakes research on the optical quality of the eye and improved imaging of its structures. She studies eye development, eye disease and linear and nonlinear optics of the eye. Campbell is known for her work on the optics of the crystalline lens, its changes with ageing and effects of visual experience on its refractive index distribution. Recently she has discovered putative optical signals to guide eye growth which follow a circadian rhythm. Campbell is a Fellow of the Association for Research in Vision and Ophthalmology, a Fellow of the Optical Society of America and a former member of OSA's Board of Directors and is a former President of the Canadian Association of Physicists. Campbell was a co-founder of Biomedical Photometrics Inc, now Huron Technologies and co-founded LumeNeuro. Campbell shared the 2004 Rank Prize in Optoelectronics for her work cited as "an initial idea (that) has been carried through to practical applications that have, or will, demonstrably benefit mankind." In 2014, she was awarded the CAP INO Medal for Outstanding Achievement in Applied Photonics in recognition of her contributions to the field of visual optics and improved imaging of structures within the eye. In 2015, she was awarded the OCUFA Status of Women Award of Distinction for her work to improve the position of academic women through organizational, policy, and educational leadership.

Gayo Diallo
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Title: Data and Knowledge Integration for Digital Public Health

Abstract: Data is nowadays routinely produced and electronic health records (EHRs) have become the standard for clinical practice. The progress in Information and Communication Technology (ICT) allows the increasing availability of tremendous non health data per-se (call data records, social networks, IoT and sensors, etc.) that enables tackling major public health issues, from post market drug monitoring to pandemic fighting or population health surveillance.

In this talk, I'll highlight some efforts in the field of AI and Public Health Data Science which rely on multidisciplinary approaches. In particular, I'll introduce knowledge graph based solutions that combine symbolic and stochastic AI. They handle heterogeneous integrated data to provide innovative digital frameworks and tools which enable public health policies and decision making.

Biography: Gayo DIALLO, HDR and PhD in Computer Sciences, is a member of the Bordeaux Laboratory of Computer Science and the Group Leader of the Computer Sciences Applied to Health research group (ERIAS) of the Bordeaux Population Health research center, INSERM 1219, a team dedicated to the design and development of methods and tools for the semantic integration of healthcare related data, in particular, for facilitating their secondary use in the context of Public Health issues. He joined University of Bordeaux, Bordeaux School of Public Health (ISPED), in 2009 after being a research assistant at City University of London (UK) and PostDoc researcher at the Laboratory of Applied Computer Sciences (LISI/ENSMA) Futuroscope Poitiers (France). He graduated from University of Grenoble Joseph Fourier in 2006 (PhD in Computer Science). His research interests include AI based approach for healthcare data and knowledge management and ICT for Development with a particular focus on the healthcare sector. He participated in various EU funded projects and authored or co-authored more than 50 peers reviewed papers. He is winner of the practical application prize of the 2015 edition of the Orange Data for Development Big Data Challenge (D4D) and the SAMPO France-Finland cooperation program in 2015 as well.

Kaan Erkorkmaz

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Title: Boosting Manufacturing through Virtualization and Intelligence

Abstract: Digitalization and distributed intelligence promise great benefits for the manufacturing industry. As full-fledged digital models, which capture in high fidelity the dynamics of processes and production machinery, become available, they enable complex manufacturing operations to be conducted, inspected, and optimized inside a virtual environment. This can circumvent the material, time, labor, and energy waste typically associated with trial and error based process development in industry. Intelligence, on the other hand, supporting advanced monitoring, model updating, optimization, and real-time control capabilities, brings key value towards furthering the productivity, part quality, and resource efficiency in manufacturing operations. Paired together, virtualization and intelligence constitute highly innovative, value enhancing, but also difficult to achieve, building blocks essential to the 4th Industrial Revolution, also referred to as 'Industry 4.0'.

This presentation will introduce case studies from on-going research at the University of Waterloo, targeting the new virtualization and intelligence capabilities for high performance manufacturing. These case studies, also undergoing validation cycles on industry-scale machines, include: machine tool and process dynamic model extraction from real-time manufacturing data; digital modeling and simulation of complex manufacturing processes, like gear machining; time-optimal trajectory planning for multi-axis processes; active damping of chatter vibrations in large machine tools using servo and/or inertial actuators.

Biography: Kaan Erkorkmaz obtained his PhD from the University of British Columbia and joined the University of Waterloo, Department of Mechanical & Mechatronics Engineering in 2004, where he now serves as Professor. Erkorkmaz conducts research on cutting mechanics, machine tool dynamics, virtual manufacturing, and high performance Computer Numerical Controls (CNC), leading successful technology co-development with, and transfer to, industry partners in the aerospace, automotive, and machine tool sectors. Parallel to his research,. Erkorkmaz teaches undergraduate and graduate courses in the areas of manufacturing, precision engineering, and automatic controls. He is recipient of the Society of Manufacturing Engineers Outstanding Young Manufacturing Engineer Award (2007), Government of Ontario Early Researcher Award (2008), InnoLecture Visiting Professorship at the University of Stuttgart (2011), and the August-Wilhelm Scheer / Global Visiting Professorships at the Technical University of Munich (2019/2020). Erkorkmaz is a Fellow of the International Academy for Production Engineering (CIRP), where he serves as Technical Secretary, and on the Editorial Committee of the CIRP Annals.

Michel Fich

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Title: ML tools for predicting maintenance requirements on a distant remote-controlled facility

Abstract: Our international CCAT-prime project team (Canada – US – Germany – Chile) is building a large telescope in Northern Chile. The site is extremely remote and at very high altitude and as a consequence there will generally be no personnel there. A wide variety of sensors will be placed throughout the structure to monitor many critical components during operations. While there will be someone remotely controlling the telescope and watching the systems on a regular basis this will not likely be continuous and many of those staffing the facility will be less experienced (e.g. graduate students and PDFs). There is a need to automatically track the system performance and alert staff if a problem occurs. However with this significant data stream from these sensors there is also the possibility to watch for changes that may predict failures in equipment. The ability to do preventative maintenance in a timely manner will likely produce cost savings and increased efficiencies in operating the facility.

Biography: A faculty member at UWaterloo since 1986, Professor Fich began building telescopes in high school. His PhD thesis work at UCalifornia (Berkeley) required the design and fabrication of a radio telescope receiver system. Since then he has been involved in numerous other astronomical instrument and telescope projects and has had a leadership role in several in the past two decades. His research publications include the first measurements of the dark matter content of our Milky Way galaxy, observations that constrain the structural evolution of galaxies, and several aspects of star formation. http://astro.uwaterloo.ca/~fich/

Vijay Ganesh

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Title: An AI Algorithm for Automated Scientific Discovery

Abstract: Automated discovery of scientific laws via computation is one of the holy grail goals of AI. While there has been considerable interest in this field in recent years, including a paper on the "Turing-Newton" challenge in the journal Nature, the state-of-the-art is still in its infancy. In this talk, I will present two new algorithms that combine machine learning and logical deduction, called Logic Guided Machine Learning (LGML) and Logic Guided Genetic Algorithms (LGGA), whose goal is to learn mathematical expressions over a given data set from some domain of science, guided by logical constraints or auxiliary truths that are known to be true of the said domain. Our methods use the principle of "corrective feedback loop", wherein, user-supplied auxiliary truths are used to guide a machine learning model in an active learning loop. Using our methods, we were able to learn up to 16 equations from the Feynman's famous books on Introduction to Physics. We conclude our talk with future directions and other ways of "combining mathematical or logical reasoning methods with machine learning" in the broad context of AI for Science.

Biography: Dr. Vijay Ganesh is an associate professor at the University of Waterloo and the Co-Director of the Waterloo Artificial Intelligence Institute. Prior to joining Waterloo in 2012, he was a research scientist at MIT (2007-2012) and completed his PhD in computer science from Stanford in 2007. Vijay's primary area of research is the theory and practice of SAT/SMT solvers aimed at AI, software engineering, security, mathematics, and physics. In this context he has led the development of many SAT/SMT solvers, most notably, STP, Z3 string, MapleSAT, and MathCheck. He has also proved several decidability and complexity results in the context of first-order theories. He has won over 25 awards, honors, and medals to-date for his research, including an ACM Impact Paper Award at ISSTA 2019, ACM Test of Time Award at CCS 2016, and a Ten-Year Most Influential Paper citation at DATE 2008. He is the Editor-in-Chief of the Springer book series "Progress in Computer Science and Applied Logic" (PCSAL) and has co-chaired many conferences, workshops, and seminars including a Simons Institute semester @ Berkeley on Boolean Satisfiability in 2021.

Stéphane Gorsse

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Title: Machine Learning Assisted Design and Development of High-entropy Alloys"

Abstract: Designing new high-performance materials is of tremendous importance to enable future technological developments. In this respect, computational thermodynamic has demonstrated its value to gain a better understanding of the relationship between atomic composition, process and microstructure, to anticipate the phases present, their volume fractions and transformation temperatures, and for guiding the development of advanced alloys with carefully designed microstructures and enhanced properties. More recently, machine learning (ML) has emerged as a technique to predict complex properties by learning from the data, and to guide the experimental effort in the most promising regions of the multi-dimensional design space.

This talk will illustrate how machine learning can help the design and development (D&D) of Refractory High Entropy Alloys (RHEAs) by bypassing the time-consuming trial-and-error method. RHEAs currently focus significant attention and efforts with the aim to overcome the temperature limit of advanced Ni-based superalloys. However, refractory alloys suffer from rapid oxidation at high temperatures. We present a ML approach to contribute to the effort being made toward the D&D of new RHEAs with better high-temperature oxidation behavior and thermo-structural properties. Our approach seeks to overcome the limitation imposed by the small size of experimental datasets. This can be achieved through out active learning cycles combining rapid experimental screening and machine learning.

Biography: SG is professor of materials science at the Institute of Condensed Matter Chemistry of Bordeaux which is a joint research unit of the French National Center for Scientific Research (CNRS), the University of Bordeaux and Bordeaux Institute of Technology.
His topics of interest include physical metallurgy, phase transformation, computational thermodynamic and alloy design.

He is the author and co-author of more than 100 papers in international peer reviewed journals.
He has been coordinator or leading researcher in EU – funded and French national research projects and projects with companies.

He gave about 50 invited lectures in international conferences and in overseas universities as invited researcher and he has received the 2018 Constellium Prize from the French Academy of Sciences for his contribution to metallurgy.

Scott Hopkins

Associate Professor
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Title: ML molecular properties from mass spectrometry data

Abstract: Conventional ML techniques have been thoroughly explored in the context of molecule discovery and have yielded encouraging results. However, despite their ease of implementation, conventional ML techniques have their drawbacks, chief among them being their demand for big data and their lack of transparency. When it comes to small molecule discovery, one can navigate these issues in advance of the application of ML by intelligent feature selection – choosing key information for ML model development – and by employing the ensemble stacking technique to create a meta-learner that accounts appropriately for the various inputs. The precision and accuracy of ML models can be further improved by including data from experimental techniques that correlate with the target property as additional model features. Differential mobility spectrometry (DMS) shows a great deal of promise in this regard because differential ion mobility is determined by molecular size and interaction potential – two fundamental properties that give rise to numerous physicochemical properties in the condensed phase. This talk will provide a brief overview of how ML and DMS may be used to determine the structures and properties of pesticides.

Biography: Scott Hopkins is an Associate Professor of chemistry at the University of Waterloo. He completed his PhD in high-resolution spectroscopy in 2006 at the University of New Brunswick, then undertook postdoctoral studies in photodissociation dynamics and gas phase cluster science at Queen's University, the University of Cambridge, and the University of Oxford where he held the Ramsay Memorial Fellowship. Scott joined the University of Waterloo in 2011 where he established a research program that focuses on determining the structures and properties of gas phase clusters. To date, he has published >80 peer-reviewed articles and has authored three patents.

Vassili Karanassios

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Title: Applications of Artificial Intelligence (AI) for Spectral Interference Correction in optical emission spectrometry and of Machine Learning for development of nano-materials for sustainable energy

Abstract: In this presentation, two topics will be covered. First, use of Artificial Neural Networks (ANNs) for spectral interference correction using a lab-scape optical spectrometer and of Deep Learning for spectral interference correction using a portable optical spectrometer and a battery-operated microplasma will be discussed [1]. And second, the application of Machine Learning (ML) for development of nano-materials for sustainable energy will be described.

Biography: Vassili Karanassios is a Professor of Chemistry at the University of Waterloo (Ontario, Canada) and a co-founder of a degree-program in nano-technology engineering at the same University. Professor Karanassios received his PhD from the Univeristy of Alberta (Edmonton Canada) and was a Post Doctoral Fellow at McGill University (Montreal, Canada). In 2009, he held a Leverhulme award in the UK where he was a visiting Professor in Chemistry (Sheffield University), an Overseas Fellow of Churchill college (Cambridge University, UK), and a visiting Professor of Engineering (Cambridge University, UK) in the Center for Advanced Photonics and Electronics (CAPE).

Professor Karanassios and his group published on microfluidics and nanofluidics, on 3D printin and on rapid prototyping, on battery-operated microplasmas, on spectral interference correction using Artificial Neural Networks (ANNs) and Deep Learning, and on smartphone-enabled data acquisition and signal-processing from a variety of sensors for *on-site* chemical analysis and (potentially) for IoT applications.

Mohammad Kohandel

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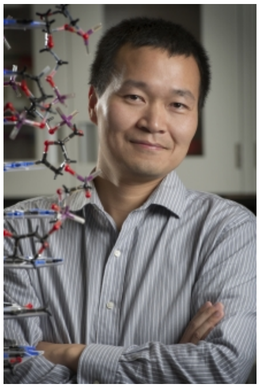
Title: AI for biomedical data

Abstract: Artificial Intelligence (AI) is a leading-edge approach for analyzing biomedical data. This talk will survey some of our recent works on applying AI to biomedical data, particularly cancer. First, I will discuss the application of physics-informed neural networks in characterizing brain tumours. Next, I will discuss how system biology and machine learning approaches can be combined to study the effectiveness of PD-1 checkpoint inhibition in ex vivo cultures. Finally, I will share our recent work on label-free identification of cancer cells.

Biography: Mohammad Kohandel is an Associate Professor at the Department of Applied Mathematics of the University of Waterloo. His Lab is currently focused on integrating experimental studies and quantitative approaches to address several problems in biomedical sciences, particularly in cancer biology. His research activities include applying existing and novel quantitative models and computational methods to study combinations of cancer therapies, nano-scale drug delivery systems, drug resistance in cancer, and quantum sensors.



Juewen Liu

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Title: Test tube evolution of DNA aptamers as biosensors

Abstract: Aptamers are single-stranded DNA oligonucleotides that can selectively bind to target molecules. They are generated by selection using a large library containing over 1014 random DNA sequences of sequences. This talk will introduce the procedures of aptamer selection and our recent work in aptamers. The implication for machine learning will also be discussed.

Biography: Dr. Juewen Liu is a professor of chemistry at the University of Waterloo and a University Research Chair. He is interested in developing DNA and aptamer-based biosensors for detecting heavy metal ions, small molecules and proteins. He received a Fred Beamish Award (2014) and a McBryde Medal (2018) from the Canadian Society for Chemistry for his contribution in bioanalytical chemistry. He is a College member of the Royal Society of Canada. He serves as a Section Editor for Biosensors & Bioelectronics, a Contributing Editor for TrAC, and is on the editorial advisory board of Langmuir. He has published over 300 papers, receiving over 30,000 citations with an H-index of 84.

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Title: DIADEM Project: Towards AI in Materials Science

Abstract: In 2021, the French government has launched priority research equipments project (PEPR in French acronym) facing key research and development challenges. In May 2021, an exploratory call was launched which got 70 applications drafts and after several selection steps, an international jury selected four projects. Among these four was DIADEM, dedicated to the **DI**scovery **A**cceleration for the **D**eployment of **E**merging **M**aterials. As a co-leader of this program together with F.Schuster (CEA), I will give some details on this program, which includes high throughput synthesis, shaping, characterization and modelling platforms for materials. The key is to assemble the data so generated in shared databases and to use these data sets for deep leaning and Artificial Intelligence tools. To start with, 9 focused projects will start in 2022 dealing with specific materials or processes. The main outcome of these projects will be to guide the platforms setting and check their efficiency. Based on this initial foundation, calls will be launched starting form 2024. All along the DIADEM 8-years life, international cooperation will be a strong commitment. Another one will be education and training aiming at convincing one third of the materials scientists to become used with AI in their everyday work by the end of DIADEM. Bordeaux University is included from the very beginning in DIADEM and the international link between our two Universities could contribute to the DIADEM internationalisation.

Biography: Mario Maglione received the Ph.D. degree from the Federal Polytechnical School of Lausanne (EPFL), Lausanne, Switzerland (1987). Following three years with IBM Zürich Laboratories, Switerland and post-doctoral positions with Mainz University, Germany, and IBM Zürich, he joined in 1988, as a Junior CNRS Scientist, the Physics Laboratory, University of Burgundy, Dijon, France. In 2000, he joined the CNRS Institute for Condensed Matter Chemistry, University of Bordeaux, Pessac, France. He has been a Director of this Institute from 2012 up to 2021. He is now a co-leader of the nationwide project DIADEM dedicated to Artificial Intelligence for Accelerated Materials Discovery. He has coauthored more than 250 papers and has been invited to 55 international conferences. His research interests are mostly concerned with the investigation of ferroelectric materials of any shape from single crystals to ceramics, nanocomposites and thin films.

Roger Melko

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Title: AI-powered Radar Sensing

Abstract: Generative models are a powerful tool in unsupervised machine learning, where the goal is to learn the unknown probability distribution that underlies a data set. Recently, it has been demonstrated that modern generative models adopted from industry are capable of reconstructing quantum states, given projective measurement data on individual qubits. These virtual reconstructions can then be studied with probes unavailable to the original experiment. In this talk I will outline the strategy for quantum state reconstruction using generative models, and show examples on real experimental data from a Rydberg atom quantum computer. I will discuss the continuing theoretical development of the field, including the exploration of powerful autoregressive models for the reconstruction of quantum states.

Biography: Roger Melko is a professor at the University of Waterloo, associate faculty at the Perimeter Institute for Theoretical Physics, and the Canada Research Chair in Computational Quantum Many-Body Physics. He received his PhD from the University of California, Santa Barbara in 2005. His research involves the development of computer strategies for the theoretical study of quantum materials, atomic matter, and quantum information systems. He was the recipient of the 2012 IUPAP Young Scientist Prize in Computational Physics, the 2016 Canadian Association of Physicists (CAP) Herzberg Medal, and the 2021 CAP Brockhouse Medal.

Sushanta Mitra

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Title: Predictive capability of water quality monitoring sensors: Need for machine learning

Abstract: In this talk, two different water quality monitoring sensors will be discussed. Firstly, to detect water-borne pathogens, such as *E. coli*, in drinking water, a detection platform was developed, called Mobile Water Kit (MWK 1.0), which shows colour change on the filter surface based on the level of pathogens present in water. A Do-It-Yourself kit, MWK 2.0, was developed using plunger-tube assembly to detect and quantify *E. coli* present in water. Secondly, to detect pesticides in water, such as carbamates and organophosphates, a Dip-and-Fold paper strip was developed that detects the concentration of pesticides through a colour change in the paper. For MWK 1.0 and 2.0, a machine learning-based mobile application platform was developed to capture the sensor image using an inbuilt smartphone camera. In such cases, the identification and classification of the captured images of the sensors were made using deep convolutional neural networks (CNN). In future, such a technique can be extended for paper-based colorimetric detection units, such as Dip-and-Fold, to provide predictive capabilities.

Biography: Sushanta Mitra is a Professor in the Department of Mechanical & Mechatronics Engineering. He serves as the Executive Director of Canada's largest nanotechnology institute – the Waterloo Institute for Nanotechnology (WIN). For his contributions in science and engineering, he is elected fellow of several professional organizations, including the Canadian Academy of Engineering, the Royal Society of Chemistry, the American Physical Society, the American Association for the Advancement of Science and a foreign fellow of both the Indian National Academy of Engineering and the National Academy of Sciences India. He has an entrepreneurial mind, being the Founder & CEO of a Canadian startup, Aquabits Inc. (on quantum computing) and a Dutch startup, SLE Enterprises B.V. (on ultra-fast encapsulation technology), supported by the University of Waterloo. His passion for working with communities in India in the water sector continues through Indian startup Earthface Analytics, for which he is a co-founder along with colleagues from IIT Kanpur and MIT USA.

Patricia Nieva

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Title: ML models for distance optimization for infectious disease-tracing (including Covid-19) using Bluetooth enabled devices

Abstract: Intelligent personal systems leverage advances in wireless, wearable, and sensing technologies, coupled with artificial intelligence (AI) algorithms, in order to facilitate effective disease transmission tracking. At the start of the COVID-19 pandemic, our work pivoted towards developing a wearable solution that can reduce the potential for significant outbreaks within our communities, while maintaining the privacy of individuals. In this talk, we will discuss advanced integrated technology-aided approaches toward the development of COVID-19 tracing methods focusing on transmission risk in different population settings. Approaches for integration of multidimensional, heterogenous data using AI will be outlined while novel transmission classification models to categorise risk will be presented.

Biography: Dr. Patricia Nieva, PhD., P.Eng., is a Professor and Deputy Chair of the Department of Mechanical and Mechatronics Engineering at the University of Waterloo. She founded and is the Director of the University of Waterloo Sensors and Integrated Microsystems Laboratory (SIMSLab). She earned her doctorate in Electrical Engineering from Northeastern University (Boston, Massachusetts) in 2004 and is an expert on microsensors, nanosensors and intelligent sensor system solutions for real-time parameter monitoring and has led extensive research in the areas of point-of-care handheld devices and smart automotive sensors. Prof. Nieva is involved in projects such as embedded sensors for in-line performance monitoring of Lithium-Ion battery cells for electric vehicles and highly sensitive, fiber-optic based salivary sensors for hormone panel testing, and handheld cardiac monitors to measure the concentration of proteins in blood commonly linked to heart attack to alert a patient’s doctor before symptoms appear. She is also currently leading the development of intelligent Bluetooth-based wearables that combine advanced sensing technologies with Artificial Intelligence (AI) to enable COVID-19 digital contact tracing and continuous health monitoring.

Sylvain Saïghi

Professor

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Title: Towards an energy sustainable AI

Abstract: In recent years, artificial intelligence (AI) has become increasingly intertwined with our daily lives. However, AI such as that currently supported by most major players in the industry like GAFAM, is decentralized to servers. Since the electricity consumption of Internet infrastructures represents 7% of the world's entire electricity production and because Internet traffic can be expected to triple every three years, we are in great need of alternative, energy-saving methods of calculation, so that the large-scale rise in AI does not lead to widespread disillusionment. In addition, embedded systems requiring AI are not necessarily permanently connected objects. The need to develop an energy-efficient material substrate for the implantation of AI in nomadic systems is becoming increasingly urgent. The development of a new hardware substrate must be accompanied by a more ambitious technological solution based on event-based computing. In this promising new computational paradigm, information is created, processed or transmitted only when a change occurs either at the level of the sensor or the calculator. Beyond reducing the amount of data, event-based computing requires fewer operations per second during the inference phase compared to classical artificial neural networks. Both characteristics make event-based computing a promising framework for designing and building energy-efficient hardware for AI.

Biography: **Sylvain Saïghi** is Professor at University of Bordeaux and head of the research group "Architecture of Silicon Neural Networks". He defended his PhD in 2004 on the design of analogue operators dedicated to silicon neurons. He has performed pioneering work in developing biologically realistic and tunable silicon neurons. He has also authored and co-authored more than 60 peer-review publications (Google scholar: 2107 citations, h-index: 20). Thanks to a Fulbright Scholar grant, he was Visiting Associate-Professor at Johns Hopkins University, Baltimore (MD), for 6 months in 2011. He was involved in the EU FACETS project and was the scientific leader for IMS Laboratory in the EU FACETS-ITN project.

Moreover, he was the coordinator of the MHANN ANR French project that aimed to build a prototype of a bio-inspired architecture, using ferroelectric memristors. Currently, he is the coordinator of the H2020 EU project ULPEC that aims at developing an ultra-low power event-based camera composed of CMOS pixels, CMOS neurons and memristive devices on the same chip. He is also currently an active partner in the NEUROTECH EU project, which intends to support the development of the European community in neuromorphic computing technologies. He recently obtained one of the chair for research on Artificial Intelligence granted by the French National Agency for research (ANR) in the frame of the French action plan for IA.

George Shaker

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Title: Low-Cost Radars and Artificial Intelligence for Advanced Sensing

Abstract: In this talk, we will present an overview of advanced sensing functionalities using low-cost radars combined with AI. We will demonstrate some applications in automotive and remote healthcare monitoring. We will discuss the design process, testing procedures, and implementation challenges.

Biography: Prof. George Shaker is the lab director of the Wireless Sensors and Devices Laboratory at the University of Waterloo where he is an (Adjunct + Research) associate professor at the Department of Electrical and Computer Engineering as well as the Department of Mechanical and Mechatronics Engineering. George is also with the University of Waterloo Schlegel Research Institute for Aging as a Research Scientist. Previously, he was an NSERC scholar at Georgia Institute of Technology. He also held multiple roles with RIM's (BlackBerry). He has co-authored over 100 peer-reviewed publications, 30 patents, and has received over 40 international research awards.

Peyton Shi

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Title: a potentially powerful tool for nano-material characterization

Abstract: Molecular beam epitaxy (MBE)-grown structures provide the footstone for many solid-state research programs and industrial applications. Further optimization of these nanomaterials can be made by studying their surface morphology, which offers direct insights into the dynamics of the crystal growth process. Surface features, such as atomic steps and hillocks, observed using atomic force microscopy (AFM), are found to vary with growth conditions. Different types of dislocations terminated at the surface show distinctive characteristics as imaged by AFM and scanning electron microscopy – electron channelling contrast imaging (SEM-ECCI). Yet, the limited processing power of human eyes and brains is unable to extract the complete information encoded in these images. Would artificial intelligence (AI) be up to the challenge?

Biography: Yinqiu (Peyton) Shi is currently a research associate working with Professor Zbig Wasilewski in the QNC-MBE Lab at the University of Waterloo. She earned her PhD degree in Physics (Nanotechnology) under Prof. Wasilewski's supervision in 2021. She graduated from the University of Toronto with a BSc in Physics in 2014. Peyton has been focusing on the epitaxial growth of InSb Quantum Well heterostructures for the experimental realization of Majorana bound states (MBS). It is a collaborative project with the Coherent Spintronics Group of the Institute for Quantum Computing (IQC), partly supported by the Transformative Quantum Technologies (TQT) program.

Laurent Simon

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Title: AI for Critical Systems: Progresses and Limits

Abstract: Despite the impressive results obtained over the last 10 years in the field of Machine Learning, errors in predictions cannot be totally eliminated. In many critical applications, producing an erroneous prediction is simply unacceptable.

In this talk, we will present reasoning-based AI that can produce verifiable proofs for its decisions. One of the main flagships of this subfield of AI is the SAT problem, which asks for the satisfiability status of a propositional logic formula. We will introduce this problem and illustrate its use on some typical problem.

We will also highlight some of the intrinsic limits of ML and SAT based approaches when it comes to producing a simple explanation of their decisions.

Biography: Professor in Computer Science at the engineering school Bordeaux INP and at the LaBRI. His main research interest is around propositional logic and the design of efficient algorithms for solving real world problems represented under this formalism (typically Constraints and SAT). He is also working on the more general frameworks Knowledge Representation and Compilation.

Rodney Smith

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Title: Empowering Spectroscopic Analysis Using the Interpretive Capabilities of ML

Abstract: By measuring the vibration of atoms in a solid, Raman spectroscopy can provide significant amounts of information regarding the structure and properties. This information, however, is often masked by the convolution of multiple phenomena. Generally, the number of vibrations is dictated by the symmetry with which atoms are distributed in the solid while the vibrational frequencies are dictated by the identity of atoms. Phase identification can therefore be carried out through a 'fingerprinting' process, where the number of vibrations and their frequency may identify the solid. This approach is not fool-proof, however, because subtle chemical and physical variations in the solid can induce changes in the spectra: introduction of structural defects such as missing atoms, physical distortion of the solid, seemingly minor changes in chemical composition, and environmental sensitivity of the sample can all affect the number and frequency of vibrations. The corollary is that subtle variations in Raman spectra can provide information on the nuanced structure of a solid. In practice, the spectra are being affected by multiple phenomena and it is challenging to isolate the effect of any single phenomenon on observed results. Our team's approach to this problem has been to apply a range of chemical characterization techniques to analyze families of samples that are nominally the same, but have some degree of systematic variation. Analysis of structure-property correlations across the series of samples may then provide insight into the major changes in structure and their effect on properties. This process is slow, requires significant depth of understanding, and is susceptible to user-bias. Machine learning techniques provide a means to facilitate the process. This presentation will introduce how the Smith Group is beginning to incorporate machine learning into our analysis routine.

Biography: Dr. Rodney Smith is an Assistant Professor at the University of Waterloo. His PhD from Memorial University of Newfoundland was followed by postdoctoral fellowships at the University of Calgary and the University of British Columbia, and an Alexander von Humboldt Research Fellowship at the Freie Universität Berlin. His research interests lie in spectroscopic analysis and in heterogeneous electrocatalysis. He has a special interest in identifying how structural imperfections affect electrochemical behavior and alter reaction mechanisms. His research team approaches the problem by correlating structural descriptors for series solid state materials to their electrochemical behavior.

Yimin Wu

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Title: Brain Inspired Computing for Artificial Intelligence

Abstract: Machine learning based artificial intelligence has profound impacts on education, economy, health care, communication, robotics, and autonomous vehicles. However, the machine learning based artificial intelligence needs to process a huge among of data. This will require better memory devices and faster processing speeds in the hardware. To address those issues, we need to use the brain inspired computing, which exhibits promising prospects for information storage and high-performance computing. The memristor device shows a small feature size (<2 nm), fast operation speeds (<1 ns), low power consumption (fJ), which is crucial for memory and computation systems. Hewlett-Packard (HP) lab prototyped a scalable 3D crossbar configuration that can realize the memory density of 1 petabit (10^{15} bits) per cm^3, by far surpassing current memory techniques. Moreover, the memristor is considered an excellent emulator of biological synapses, which may revolutionize the current computation capacity with neuromorphic computing. Due to the requirement of the memristor-based techniques, some aspects are worth further investigation for memory and neuromorphic computing, including volatile/non-volatile data storage, artificial neurons, and artificial synapse. Here, the progress of advanced memory and neuromorphic computing in my team will be discussed. Particularly, a versatile memristor for advanced memory and neuromorphic computing for pattern recognition has been developed. Beside, progress has also been obtained on artificial synapses and flexible neuromorphic computing. The results will facilitate the brain-inspired computing for artificial intelligence.

Biography: Dr. Yimin Wu is an assistant Professor in the Department of Mechanical and Mechatronics Engineering and Waterloo Institute of Nanotechnology (WIN), Director of Materials Interfaces Foundry, at the University of Waterloo. Dr. Wu received his DPhil degree in Materials from the University of Oxford on 2D electronics in 2013. Then, he worked as a SinBeRise Postdoctoral Fellow at the University of California, Berkeley, and Lawrence Berkeley National Laboratory. Prior to joining the faculty at Waterloo in 2019, he was focusing on the advanced catalysts and battery research in the Center for Nanoscale Materials and Joint Center for Energy Storage Research (JCESR), Argonne National Laboratory and worked as a research assistant professor at University of Illinois, USA. He has authored and co-authored more than 50 peer-reviewed journal papers, which includes Nature, Nature Energy, Nature communications. He is also listed as a primary inventor on 1 US/international patent. His research has been highlighted by Canadian Press, CBC news, the Independent, BNN Bloomberg, Fast Company, and French Science Magazine. He has been awarded more than 10 awards including Nanoscale Emerging Investigator (2022), WIN research leaders award (2020), MIT Technical Review Innovators Under 35 Award Finalist (2020), SinBeRise Postdoctoral Fellowship at the University of California, Berkeley (2013), UK EPRSC Doctoral Prize (2012).Wu has delivered over 25 invited lectures across the world in last 5 years. His research group has received funding from federal and provincial government agencies (Natural Science and Engineering Research Council of Canada, Canadian Foundation for Innovation, National Research Council Canada, Ontario Center of Excellence, and MITACS). https://uwaterloo.ca/materials-interface-foundry/

Frank Zhu
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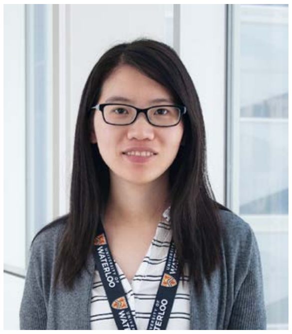
Title: PlasticNet – Deep learning for automatic microplastic recognition in water via FT-IR Spectroscopy

Abstract: The recognition of microplastics (MPs) in environmental samples via Fourier transform infrared spectroscopy (FT-IR) is challenging due to a plethora of factors such as the presence of plasticizers, weathering, and contamination that can lead to significant variances in measured spectra for a given type of plastic. Conventional library search approaches proposed in literature rely on comparing the observed spectrum with spectra in reference libraries, and thus significant spectra variances can lead to recognition errors when leveraging such approaches. Motivated to tackle this challenge, this study explores the feasibility of leveraging deep learning for automatic MP recognition via FT-IR spectroscopy. More specifically, a deep convolution neural network (CNN) architecture, referred to here as PlasticNet, is introduced for the purpose of automatic MP recognition. PlasticNet was trained on a large corpus of FT-IR spectra of different plastic types in order to learn discriminative spectral features characterizing each plastic type. Experimental results showed that 1) PlasticNet was capable of different between 11 types of common plastic in wastewater particles from a sample in an effective and efficient manner; 2) The PlasticNet correctly identified particles that were not recognized via a library search technique and at a faster recognition speed as well; 3) The PlasticNet showed good performance in recognizing spectra with variation. The PlasticNet was employed to recognize MPs that were composed of 5 types of Polypropylene (PP) and 6 types of Polyethylene (PE) that had either experienced weathering or contained additives including UV stabilizer, anti-oxidants, process-scavengers, fire retardants and dyes. These spectra had additional peaks compared with the spectra of pure PP and PE MPs. Despite this, PlasticNet achieved 90%+ success in recognizing MPs in the test dataset thereby demonstrating that deep learning can resolve spectral variation in spite of the presence of additional peaks.

Biography: I am Ph.D. student from the department of civil and environmental engineering. My Ph.D. project focuses on the fate and transport of microplastics(MPs) in wastewater treatment plants. I aim to develop novel analytical methods leveraging deep learning and image analysis for the rapid and accurate detection of microplastics in wastewater samples. I specially focus on the use of deep learning for the recognition of spectra of MPs in environmental samples that vary significantly from the spectra of pure polymers.



Qinqin Zhu

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Title: Dynamic Latent Variable Analytics for Inferential Sensor Modeling and Supervised Monitoring

Abstract: With the advent of Industry 4.0, industrial data can be collected at very high sampling rates, leading to more complicated relation between process and quality variables. To extract valuable information from these variables and avoid the curse of dimensionality, multivariate latent variable methods (LVM) are widely used, such as partial least squares (PLS), canonical correlation analysis (CCA) and latent variable regression (LVR). These models obtain satisfactory modeling and monitoring performance; however, their static assumption constrains their applicability in actual dynamic systems. Several dynamic variants were proposed to extract temporal information from the data, which still have some limitations such as incomplete exploitation of quality information.

In this presentation, a series of dynamic auto regressive LVM (DALVM) algorithms are proposed to fully exploit the valuable information of both process and quality variables. DALVM aims to maximize the dynamic relations between current quality samples and past process and quality samples, and to achieve consistency, an auto-regressive exogenous (ARX) model is designed in the inner model. In DALVM, in addition to the auto-regressive relations of quality variables, the cross-correlations between **X** and **Y** are also constructed. Further, a DALVM-based comprehensive monitoring scheme is proposed. Two industrial dataset, Tennessee Eastman process and the three-phase flow facility, are used to illustrate the advantages of the proposed algorithms.

Biography: Prof. Qinqin Zhu is an assistant professor in the department of Chemical Engineering at the University of Waterloo. She is also a faculty member in the Waterloo Artificial Intelligence Institute (Waterloo.AI), Waterloo Institute for Nanotechnology (WIN), and Waterloo Institute for Sustainable Energy (WISE). Prof. Zhu received her PhD degree from the Chemical Engineering department at the University of Southern California. Prior to UW, she worked as a senior research scientist at Facebook Inc. in the United States. Prof. Zhu's research mainly focuses on developing advanced statistical machine learning methods, process data analytics techniques and optimization algorithms in the era of big data with applications to statistical process monitoring and fault diagnosis. Her research addresses theoretical challenges and problems of practical importance in the area of process systems engineering. By leveraging the power of mathematical modeling and optimization, her group strives to develop advanced multivariate statistical analysis algorithms that enhance decision

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