HARRISON—MACRAE FAMILY LECTURE

The Harrison – MacRae Family Lecture Series was established through the generosity of the estate of the late John H. Harrison (Queen's B. Comm., 1949) and Elizabeth (Betty) Harrison (nee MacRae, Queen's B.A., 1949). For over a century the Harrison - MacRae family has attended Queen's University and has shown a distinct enthusiasm for the arts and sciences. Elizabeth Harrison is the daughter of Queen's graduates Alex E. MacRae (B.Sc. Chem. Eng., 1914) and Irene McAllister (B.Sc. Math & Physics, 1914), and sister to Queen's graduates Jean C. Doherty (B.A. 1939), Donalda I. Beattie (B.A. 1939), Marion E. Bradley (B.A. 1946), and brother Robert A. MacRae (B.Sc. Chem. Eng., 1954). Their son Ian Harrison (Queen's B.Sc. Chem. Phys., 1981) is a Professor of Chemistry at the University of Virginia. Numerous children, grandchildren and great grandchildren have likewise attended Queen's University. In recognition of their long affinity for Queen's, this lecture series will feature seminars by distinguished scientists on topics within the fields of chemical physics or physical chemistry.

PREVIOUS HARRISON-MACRAE LECTURERS

2020 • U. Schollwöck

2019 • I. Harrison

2019 • P. Willis

2019 • C. Adachi

2018 • B. Bayram

2018 • V. Batista

2016 • A. Aspuru-Guzik

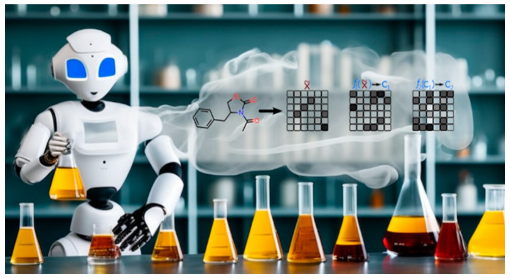
Queen's Chemistry

Department of Chemistry
Queen's University

is honoured to host the 2024 Harrison—MacRae Lecturer:

Prof. Olexandr Isayev

Carnegie Mellon University



"Accelerating Molecular Design with Machine Learning and AI"

Friday, April 26, 2024
11:30 AM
Room 117, Chernoff Hall

and

"Tutorial on Neural Networks for Quantum Mechanical (QM) Calculations"

1:30 PM
Room STI A, Stirling

PROF. OLEXANDR ISAYEV

Prof. Olexandr Isayev
Department of Chemistry
Carnegie Mellon University
Pittsburgh, U.S.

Olexandr Isayev is an Associate Professor at the Department of Chemistry at Carnegie Mellon University (CMU). He received his Ph.D. in computational chemistry in 2008. He was a Postdoctoral Research Fellow at the Case Western Reserve University and a scientist at the government research lab. Before joining CMU, he was a faculty at the Eshelman School of Pharmacy of the University of North Carolina at Chapel Hill. Olexandr received the “Emerging Technology Award” from the American Chemical Society (ACS) and the GPU computing award from NVIDIA Corp. Olexandr is 2023 Scialog Fellow and Associate Editor for ACS Journal of Chemical Information and Modeling. The research in his lab focuses on connecting artificial intelligence (AI) with chemical sciences.

SELECTED RECENT PUBLICATIONS

- D. Anstine, R. Zubatyuk, O. Isayev. AIMNet2: A Neural Network Potential to Meet your Neutral, Charged, Organic, and Elemental-Organic Needs. ChemRxiv Preprint 2024. https://doi.org/10.26434/chemrxiv-2023-296ch
- D. M. Anstine and O. Isayev. Generative Models as an Emerging Paradigm in the Chemical Sciences. *J. Am. Chem. Soc.* 2023, 145, 16, 8736–8750. https://doi.org/10.1021/jacs.2c13467
- M. Reis, F. Gusev, N. Taylor, S. H. Chung, M. Verber, Y. Lee, O. Isayev, and F. Leibfarth. Machine Learning-Guided Discovery of ^{19}F MRI Agents Enabled by Automated Copolymer Synthesis. *J. Amer. Chem. Soc.* 2021, 143, 17677. https://pubs.acs.org/doi/10.1021/jacs.1c08181.
- T. Zubatiuk, O. Isayev. Development of Multimodal Machine Learning Potentials: Toward a Physics-Aware Artificial Intelligence. *Accounts of Chemical Research.* 2021, 54, 1575-1585. https://doi.org/10.1021/acs.accounts.0c00868
- M. Popova, O. Isayev, A. Tropsha. Deep Reinforcement Learning for de-novo Drug Design. *Science Adv.* 2018 4 (7), eaap7885. https://www.science.org/doi/10.1126/sciadv.aap7885
- K. T Butler, D. W Davies, H. Cartwright, O. Isayev, A. Walsh. Machine learning for molecular and materials science. *Nature*. 2018, 559, 547–555. https://www.nature.com/articles/s41586-018-0337-2