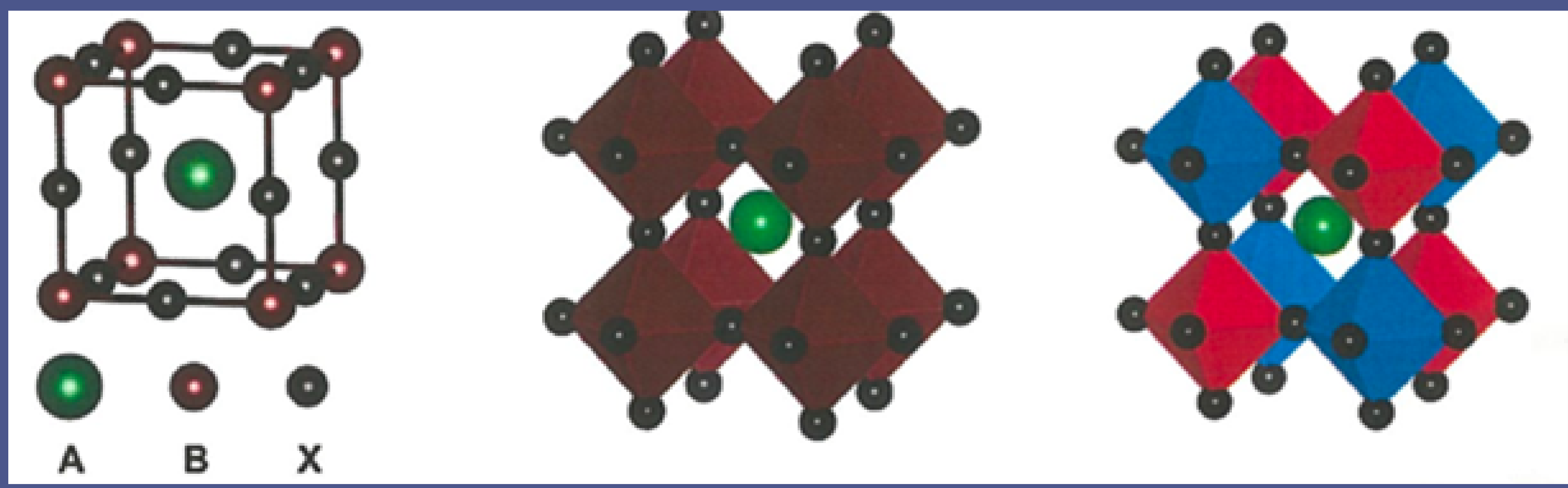
Chemical & Physical Sciences

UNIVERSITY OF TORONTO

MISSISSAUGA

COLLOQUIUM SEMINAR SERIES

INSIGHTS INTO ATOMIC-LEVEL STRUCTURE AND DYNAMICS IN PEROVSKITE AND PEROVSKITE-INSPIRED MATERIALS FROM SOLID-STATE AND DYNAMIC NUCLEAR POLARIZATION NMR SPECTROSCOPY



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Transitioning from legacy fossil fuels to alternatives will require a multipronged approach to accessing energy harvesting, storage, and reducing consumption. One emerging class of materials that satisfies these societal needs is perovskite or metal halide perovskite-like compounds. The most ubiquitous perovskite in the current literature is methylammonium lead iodide ($MAPbI_3$). However, this area is rapidly evolving due to the immense chemical and synthetic variability possible at the A, B, or X sites and the dimensionality. While perovskites are defect tolerant, they suffer from phase segregation or changes and decomposition, often associated with moisture or heat. This unusual behaviour for hybrid and inorganic materials is rooted in intrinsic dynamics and local structural disorder, which is difficult to track via traditional diffraction approaches. Solid-state nuclear magnetic resonance (NMR) spectroscopy is a robust, non-destructive, and nucleus-specific characterization method for local- and medium-range atomic structure and dynamics that can fill in the missing clues needed to industrialize these materials for the future.

This presentation touches upon an interdisciplinary approach using physical, solid-state and materials chemistry to solve these materials' complex structure, dynamics, and structure-property relationships. Specifically, this talk will focus on our use of solid-state NMR, high-field dynamic nuclear polarization (DNP), nuclear quadrupole resonance (NQR) and electron paramagnetic resonance (EPR) as robust analytical characterization spectroscopies. Recent findings from our lab in solid-solution behaviour, ion doping and substitution and decomposition pathways, developed by exploring exotic heavy metals (^{207}Pb, ^{119}Sn) and challenging quadrupolar (^{73}Ge, ^{133}Cs, $^{121/123}Sb$, $^{113/115}In$, ^{209}Bi, $^{35/37}Cl$, $^{79/81}Br$, etc.) nuclei, will be discussed. Phase changes and cation, anion, or octahedral dynamics, investigated via in situ relaxometry NMR measurements and variable-temperature NMR, which can range between 95 and 800 K, are discussed. Furthermore, complementary results from quantum chemical computations, X-ray diffraction, and scanning electron microscopy enable us to provide a complete structural picture of their short-, medium-, and long-range structure.

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featuring

Prof. Vladimir K. Michaelis

Wednesday, February 15, 2022 | 3:30pm

Location: CCT2150