TRENT UNIVERSITY

PHYSICS & ASTRONOMY SEMINAR SERIES

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Wednesday, November 8, 2023
11:00 a.m. to 11:50 a.m. in ENW 115

Unusual electronic properties of lead-halide perovskites: structural dynamics, surface states and defects

Abstract:

Hybrid organic and inorganic single-crystal lead-halide perovskites (for instance, $(CH_3NH_3)PbI_3$ or $CsPbI_3$) are one of the hottest topics in contemporary materials science. The initial interest of the community was motivated by the application of lead-halide perovskites as an active material in solar cells and later expanded to other optoelectronic devices. The material combines several attractive characteristics: relatively straightforward fabrication, tolerance to defects, a direct band gap character, and a long lifetime of charge carriers. Usually, the last two characteristics are mutually exclusive. Contrary to conventional solar cell materials, surfaces and grain boundaries in lead-halide perovskites are not a significant source of deep electronic traps. As a result, the efficiency of polycrystalline halide perovskite solar cells already surpasses that of the best polycrystaline silicon cells. In this presentation, I will shed light on the possible origin of these unusual characteristics by employing ab initio electronic structure calculations.