## HIGHLANDS IN CHEMISTRY SEMINAR SERIES



MARCH 15, 2024

2:30PM

HAHN HALL NORTH 140

FACULTY HOST: LOUIS MADSEN/FENG LIN

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"Molecular Scale Modeling of Battery Electrolytes and Interfaces"

Supply chain issues due to heterogenous distribution of essential materials for lithium-ion batteries call for exploration of alternative battery chemistries. Aqueous zinc and non-aqueous magnesium batteries are considered as promising complementary energy storage technologies, especially for grid storage applications. In this presentation, I will provide an overview of our recent molecular dynamics simulations and DFT studies of the aqueous zinc, non-aqueous magnesium electrolytes and lithium-ion batteries with a focus on understanding of the electrolyte structure, transport and hints on tailoring the solid electrolyte interphase (SEI) and cathode electrolyte interphase (CEI) composition to improve reversibility of cell cycling including improved low temperature performance and safety.

