# Department of Materials Science and Engineering Seminar Series 2024

# First-Principles Multiscale Investigations of Functional Coating Materials for Energy Materials


## Chen Hengning


### Date and time: 10th Oct 2024 (Thurs) 11:00 am

### Venue: E1-06-08 SEMINAR ROOM, E1-06-09

# Abstract


Developing and optimizing advanced energy storage devices, particularly lithium-ion batteries (LIBs) and all-solid-state batteries (ASSBs), has become critical in addressing the growing demand for high-performance and safe energy storage solutions. However, challenges at the positive electrode-electrolyte interface, including chemical/electrochemical instability and high charge-transfer resistance, continue to impede overall battery efficiency and longevity. To address these critical issues, this research investigates promising halide electrolyte and functional coating materials, lithium niobates, and lithium tantalates. We first uncover the role of stacking faults in facilitating Li-ion transport within $Li_3YCl_6$ by lowering the migration barriers and generating additional interlayer channels. Subsequently, through a comprehensive study of chemical and electrochemical stability, defect analysis, and modeling of Li-ion transport, we reveal the multiphasic nature of crystalline lithium niobates and lithium tantalates. Notably, we underscore the critical role of defect complexes in phase stabilization and facilitating Li-ion transport. Contrary to the previously conceived $LiNbO_3$ and $LiTaO_3$, we find that secondary phases, such as $Li_3NbO_4$ and $Li_3TaO_4$, also play crucial functional roles within the coating layer. To optimize these coating materials, we further investigate the mixing of Nb and Ta in the Li-Nb-Ta-O system. Combining first-principles calculations with statistical mechanics approaches, we predict the temperature-composition phase diagram for Li-Nb-Ta-O in conjunction with Monte Carlo simulations, providing valuable insights for tailoring coating properties.

# Biography

Chen Hengning received her B.Sc. degree from University of Chinese Academy of Sciences in 2020. She is currently a Ph.D. candidate under the supervision of Asst. Prof. Pieremanuele Canepa. Her research employs multiscale first-principles simulations to investigate the mechanism and optimize the properties of functional coating materials for batteries.

**Please join us!**

HOST: Assoc Prof Andreeva-Baeumler Daria