

## Joint seminar of the NPI of the CAS

29. 1. 2026

**Charles Hervoches, Ph.D. (DNIM NPI): *Probing structure–property relationships in energy materials using advanced diffraction techniques***

Abstract:

Accurate, non-destructive structure determination is essential for rationally engineering energy materials. In this seminar we survey state-of-the-art diffraction techniques—X-ray, neutron, synchrotron, TEM, PDF, and EXAFS—alongside complementary computational modeling, and illustrate their application to three systems: Bi-based oxide-ion conductors, proton-conducting  $\text{La}_{5.6}\text{WO}_{12-\delta}$ , and the magnetic–electric (ME)  $\text{A}_4\text{M}_2\text{O}_9$  family. Together, these studies demonstrate that bridging long-range order with local dynamic disorder—achieved only through complementary diffraction techniques and theory—provides the critical structure–property map needed to design next-generation ionic conductors and magnetoelectric devices.