

Joint seminar of the NPI of the CAS

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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.