



22<sup>nd</sup> International Conference on  
Diffusion in Solids and Liquids  
22 TO 26 JUNE 2026 | RHODES, GREECE

## ABSTRACT:

### Multimodal Atomistic Structural Refinements of Functional Materials

I. Levin

Materials Measurement Science Division

National Institute of Standards and Technology, Gaithersburg, MD, USA

Functional materials often exhibit structural complexity across multiple length scales, where local disorder, chemical heterogeneity, and correlated atomic displacements significantly influence macroscopic properties. Traditional crystallographic methods, which focus on the average structure, cannot fully capture these nanoscale correlations. Overcoming this challenge requires experimental and analytical strategies that integrate complementary structural information from various probes.

In this talk, I will discuss multimodal atomistic structural refinements, an emerging method that refines large atomistic configurations using several experimental datasets. By combining inputs from techniques sensitive to different structural and chemical aspects—such as neutron and X-ray total scattering, diffuse scattering, and element-specific X-ray absorption spectroscopy—this approach reconstructs correlated atomic displacements and chemical ordering patterns over nanometer length scales. Integrating diverse datasets within a single refinement framework allows access to structural information unattainable from any single technique. This strategy enables the concurrent description of average structure, local distortions, and nanoscale correlations within one model, providing a coherent view of structural complexity.

As an example, I will present recent multimodal refinements of the relaxor ferroelectric  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3\text{-PbTiO}_3$ . The simultaneous analysis of neutron and X-ray total scattering, diffuse scattering, and X-ray absorption data reveals a network of correlated polar displacements that forms swirling polarization textures with vortex-like defects, rather than isolated polar nanoregions. These polarization vortices emerge from the interplay between nanoscale compositional heterogeneity, local strain fields, and electrostatic interactions.

I will also discuss the implications of our findings for understanding correlated disorder and emergent nanoscale phenomena across a broader range of functional materials.