# Accelerating atomic-scale characterization by combining theory and AI/ML*

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## Abstract

At DOE Scientific User Facilities, multi-modal x-ray, electron, laser, and scanning probes, as well as computational modeling tools, have now become indispensable in providing complementary atomic-scale information. However, determining where atomic-scale structure information from scattering, microscopy, spectroscopy, or computational modeling alone remains a substantial challenge. I will discuss our efforts in using a theory-informed artificial intelligence and machine learning (AI/ML) framework to allow researchers to extract atomic-level information from experimental characterization data. Examples include x-ray core level spectroscopy, scanning transmission electron microscopy, and scanning tunneling microscopy.

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