

# High-Resolution Crystal Imaging via Bragg Diffraction and Modeling

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## Executive Statement:

PRAMMol (Phase Retrieval with Atomic Modeling and Molecular Dynamics) is a groundbreaking coherent diffraction imaging algorithm designed for atomic resolution from diffraction patterns, using molecular dynamics and maximum likelihood estimation.

## Description:

PRAMMol (Phase Retrieval with Atomic Modeling and Molecular Dynamics) is an innovative imaging algorithm that enhances Bragg Coherent Diffraction Imaging (BCDI) to achieve atomic scale resolution. It integrates molecular dynamics and maximum likelihood estimation into a physics-based iterative phase retrieval process. This novel approach significantly reduces computational costs and overcomes the limitations of traditional phase retrieval methods, facilitating highly accurate reconstructions of atomic positions from diffraction patterns.

## Key Advantages:

- Enables atomic scale resolution with lower time-integrated photon flux compared to traditional methods.
- Reduces computational costs and search space in the phase retrieval problem through a physics-based iterative approach.
- Expands the potential applications of x-ray imaging in material science and biology.
- Supports real-time imaging of materials at the atomic level, complementing upgrades to synchrotron facilities.
- Validated through simulations, demonstrating high precision in reconstructing complex atomic structures.

### **Problems Solved:**

- Overcomes the limitations and high computational costs of traditional phase retrieval methods.
- Achieves high-resolution imaging without the need for extremely high photon flux.
- Facilitates precise imaging of complex atomic configurations, such as grains and grain boundaries in materials.

### **Market Applications:**

- Advanced battery materials analysis.
- Protein crystallography for biological research.
- Material science, particularly for examining crystalline structures.
- Real-time atomic level imaging of various materials.