PAIR DISTRIBUTION FUNCTION (PDF)

NSLS-II Diffraction & In Situ Scattering Program

BROOKHAVEN NATIONAL LABORATORY

NATIONAL SYNCHROTRON LIGHT SOURCE II

SCIENTIFIC SCOPE

PDF is the dedicated Pair Distribution Function beamline at the NSLSII. The atomic pair distribution function yields a histogram of atom-atom pair distances describing the structure on different length-scales. PDF allows studies of nanoscale fluctuations in complex materials under real operating conditions. High flux and fast area detectors available at the beamline facilitate studies of the evolution of materials during synthesis.

BEAMLINE CHARACTERISTICS

TECHNIQUES:

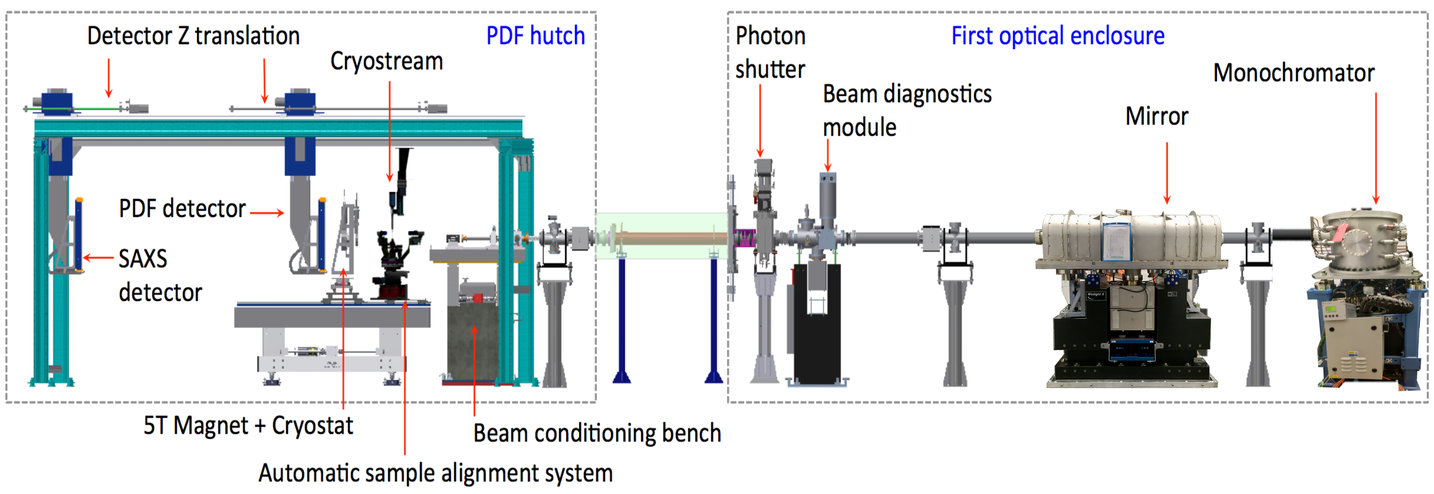
- Atomic Pair Distribution Function
- Small-Angle X-ray Scattering
- Wide Angle X-ray Scattering

ENDSTATION DETAILS:

- Two large area detectors
- A wide variety of sample environments
- Gas handling system

PDF ENABLES:

- Studies of nanoscale structural fluctuations in strongly correlated materials
- In-situ or operando characterization of catalysts
- Studies of the local structure of batteries during charging and discharging cycles
- Studies of structure-property relationships in functional nanomaterials



Schematic layout of the PDF beamline: PDF uses a horizontally focusing side bounce monochromator to select the operational energy. The vertical focusing of the beam is achieved by using a 1.5 m long bent mirror.

Overview

PORT: 28-ID-1

SOURCE: Damping Wiggler (DW100)

ENERGIES: 39, 64, 75 and 117 keV

ENERGY RESOLUTION: $\Delta E/E = 10^{-2} - 2 \times 10^{-3}$

FOCUSED BEAM SIZE: ~ 0.1 (v) X 0.25(h) mm

BEAMLINE STATUS: Under Construction

WEBSITE: www.bnl.gov/nsls2/beamline/28-ID-1

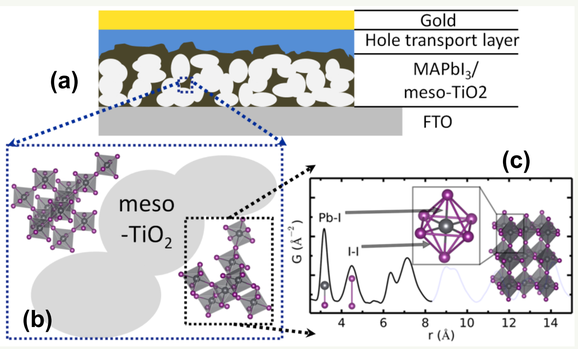
Beamline Staff

Milinda Abeykoon

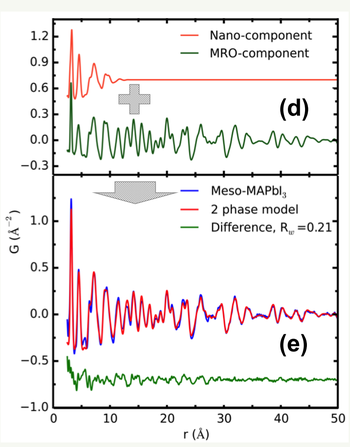
Lead Beamline Scientist

SCIENTIFIC APPLICATIONS

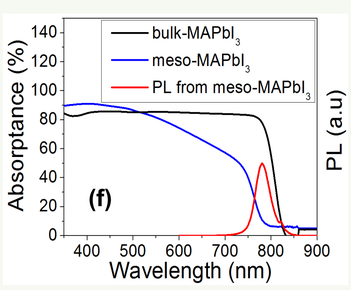
Methyl-ammonium Lead Iodide in high-performance Perovskite solar cells



Schematic diagrams of **(a)** A perovskite-based solar cell, and **(b)** Possible configurations of meso-$MAPbI_3$ within the active layer of the cell. **(c)** PDF of $MAPbI_3$ providing quantitative information on all atom-atom correlation lengths.



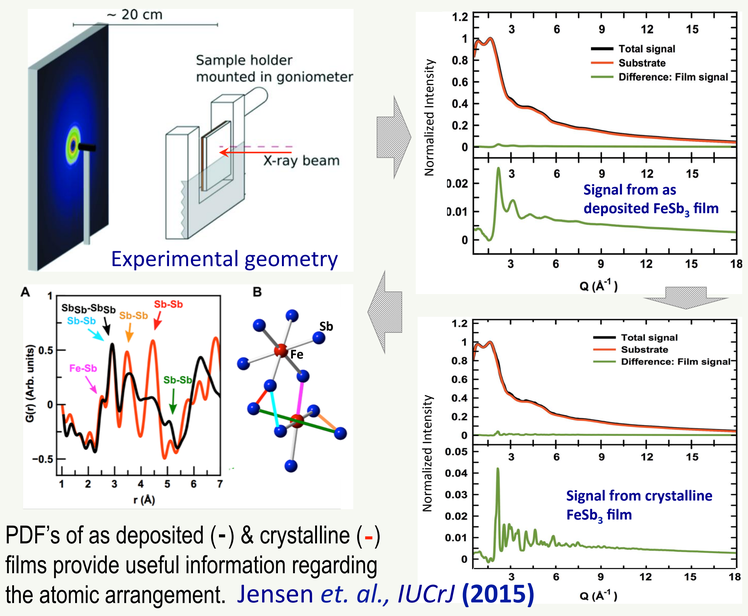
(d) PDF of the meso-$MAPbI_3$ reveals disordered nanostructured and medium range ordered (MRO) phases. **(e)** Resulting 2- Phase model fit



(f) Due to the nature of this atomic arrangement, optical absorption (blue) and photoluminescence (red) spectra illustrates strongly modified optical properties relative to the pure bulk material (black). Choi *et. al.*, Nano Lett., 14 (1), pp 127–133, **(2014)**

Thin film PDF (tPDF)

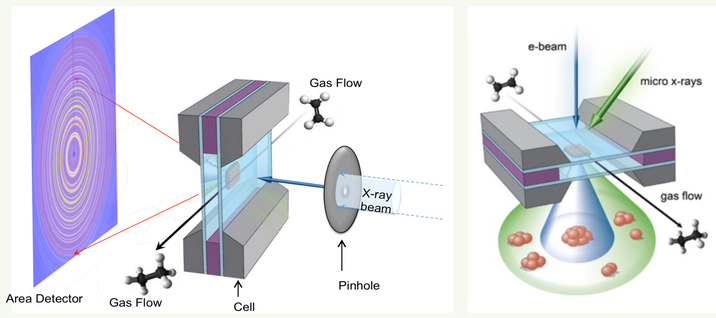
PDF is a great tool to study the crystal structure of thin films.



PDF's of as deposited (-) & crystalline (-) films provide useful information regarding the atomic arrangement. Jensen *et. al.*, *IUCrJ* **(2015)**

Correlative operando X-ray PDF and electron microscopy of catalysts

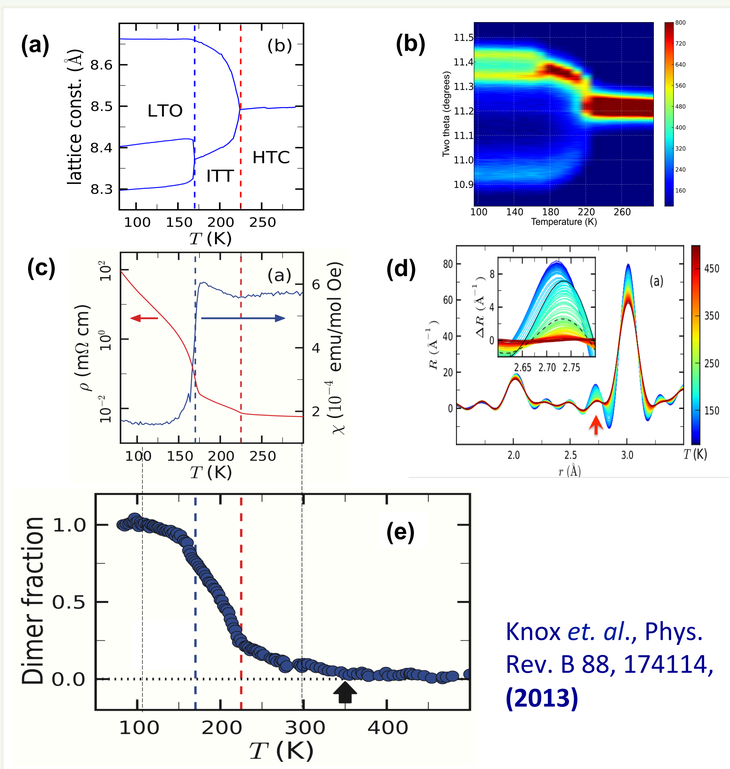
A new TEM cell developed at BNL (Stach *et. al.*) enables X-ray PDF and electron microscopic studies of the active structure and local morphology of the same catalysts operating in the the same reactive environments.



PDF setup TEM setup

Local structural response to the electronic state of materials

Two-stage metal insulator phase transition occurs in $LiRh_2O_4$ with known Rh^{4+}-Rh^{4+} dimers in the low-T phase (LTO). For the first time, high r-resolution PDF studies confirmed the existence of dimers in all three phases.



Knox *et. al.*, Phys. Rev. B 88, 174114, **(2013)**

T-evolution of; **(a)** Lattice constants, **(b)** A selected Bragg peak, **(c)** resistivity (red), magnetic susceptibility (blue), and **(d)** Dimer distance PDF peak (↑). The inset of **(d)** shows Differential PDF's at the dimer distance obtained by subtracting the 500 K PDF from each PDF. Black lines at 170 K (solid), and 225 K (dashed) denote differential PDF's at the phase transition temperatures. **(e)** T-evolution of the integrated intensity of the dimer peak normalized to its low-T value represents the dimer fraction.