

XAFS 2021
Short course: introduction to X-ray Absorption Fine Structure
Brookhaven National Laboratory, November 17-19 2021

Instructors:

Grant Bunker (IIT), Amani Ebrahim (SBU), Anatoly Frenkel (SBU/BNL), Joshua Kas (UW), Shelly Kelly (ANL), Yuanyuan Li (SBU), Yang Liu (SBU), Nicholas Marcella (SBU), David Sprouster (SBU), Fernando Vila (UW)

Pre-requisite (self-study):

Synchrotron sources, detectors – G. Bunker (Link will be provided)

November 17 (Wednesday)

Part 1. Lectures:

9am: Introduction - A. Frenkel
9:30 am Introduction and overview of XAFS – A. Frenkel
10:30 am Sample preparation- G. Bunker.
11:30-12 pm *Break*
12pm Theory and calculation of X-ray spectra with FEFF – J. Kas
1:30-2:30 pm *Break*
2:30 pm Concepts of EXAFS data analysis– G. Bunker

Part 2. XAFS Fundamentals: Questions and Answers

3:30-5 pm Questions that come in real time or prepared in advance. Questions may include discussing a particular project or structure or experimental planning. Main room. All instructors.

November 18 (Thursday)

Part 1. Lectures:

9 am XANES data analysis with FEFF (demo)– F. Vila
10 am XAFS data processing with Demeter/Athena: S. Kelly
11-11:30 am *Break*
EXAFS data analysis with Demeter/Artemis: S. Kelly
1-2 pm *Break*
2-3:30 pm Application of XAFS to catalysts – A. Frenkel

Part 2. Problem solving strategies: Questions and Answers

3:30-5 pm Questions that come in real time or prepared in advance. Questions may include discussing a particular project, structure, data, analysis strategy. Main room. All instructors.

November 19 (Friday)

Solving open ended problems/projects/ proposed by instructors and/or participants.

Breakout rooms, up to 8 participants per room, organized according to the topic (XANES modeling or EXAFS analysis), moderated by all instructors.

9-9:30 am Setup of breakout rooms

9:30-11 am Breakouts

Break

11:30-1 pm Breakouts

Break

2-3:00 pm Breakouts

Break

3:30-5 pm Breakouts

5 pm: Adjourn