

Data Analysis and Modeling of XANES and EXAFS Spectra:

Applications to Nanomaterials

Medical Building 490, Brookhaven Avenue

Workshop Agenda

Wednesday, November 1		
9:00 am	<i>Welcoming remarks</i>	A. Frenkel
9:10 am	<i>Introduction and overview of XAFS</i>	A. Frenkel
9:40 am	<i>Obtaining 3D structure from EXAFS spectra</i>	J. Timosenko
	<i>Part 1: Wavelet transform analysis</i>	
10:40 am	<u>Coffee break</u>	
11:00 am	<i>Obtaining 3D structure from EXAFS spectra</i>	J. Timosenko
	<i>Part 2: Reverse Monte Carlo simulations and evolutionary algorithm</i>	
12:00 pm	<i>The use of Molecular Dynamics simulations for the interpretation of EXAFS spectra</i> <i>Part 1</i>	A. Kuzmin
1:00 pm	<u>Lunch</u>	
2:00 pm	<i>Group Photo</i>	
2:20 pm	<i>The use of Molecular Dynamics simulations for the interpretation of EXAFS spectra</i> <i>Part 2</i>	A. Kuzmin
3:10 pm	<i>RMC refinements of 3D local atomic structures using multiple data sets Part 1</i>	V. Krayzman
4:00 pm	<u>Coffee break</u>	
4:30 pm	<i>RMC refinements of 3D local atomic structures using multiple data sets. Part 2</i>	V. Krayzman
6:00pm	<u>Dinner</u>	

Thursday, November 2		
9:00 am	<i>Overview of Athena and Artemis (Demeter data analysis package)</i>	A. Frenkel
9:40 am	<i>Software demonstration Part 1: Wavelet transform analysis</i>	J. Timosenko
10:40 am	<u>Coffee break</u>	
11:00 am	<i>Software demonstration Part 2: Reverse Monte Carlo simulations and evolutionary algorithm</i>	J. Timosenko
12:00 pm	<i>Software demonstration for Molecular Dynamics simulations of EXAFS spectra. Part 1</i>	A. Kuzmin
1:00 pm	<u>Lunch</u>	
2:20 pm	<i>Software demonstration for Molecular Dynamics simulations of EXAFS spectra. Part 2</i>	A. Kuzmin
3:10 pm	<i>Software demonstration. Part 1</i>	V. Krayzman
4:00 pm	<u>Coffee break</u>	
4:30 pm	<i>Software demonstration. Part 2</i>	V. Krayzman
6:00 pm	<u>Dinner</u>	

Friday, November 3		
9:00 am	Data analysis practicum	Instructors: J. Timosenko, A. Kuzmin, V. Krayzman, Y. Li, H. Singh, A. Frenkel
12:00 pm	<u>Lunch</u>	
1:00 pm	Data analysis practicum	Instructors: J. Timosenko, A. Kuzmin, V. Krayzman, Y. Li, H. Singh, A. Frenkel
5:00 pm	<u>Adjourn</u>	