

Short Course on X-ray Absorption Fine Structure: Advanced topics in data analysis and modeling

Tentative Agenda (time slots may change)

Wednesday, Nov 1

- 9:00am **A. Frenkel** *Welcoming remarks*
- 9:20am **J. G. Chen** *Synchrotron Catalysis Consortium (SCC)*
- 9:50am **A. Frenkel** *Introduction and overview of XAFS*
- 10:30am Break
- 11:00am **K. Lomachenko** *XAS experiment: maximizing the data quality*
- 12:00pm Adjourn for lunch
- 1:00pm **A. Kuzmin** *The use of Molecular Dynamics simulations for the interpretation of EXAFS spectra*
- 2:00pm **J. Timoshenko** *Obtaining 3D structure from EXAFS spectra.*
Part 1: Wavelet transform analysis
- 2:30pm **J. Timoshenko** *Obtaining 3D structure from EXAFS spectra.*
Part 2: Reverse Monte Carlo simulations and evolutionary algorithm
- 3:30pm Break
- 4:00pm **K. Lomachenko** *Resolving spectral mixtures: linear combination fitting, principal component analysis and MCR-ALS*
- 5:00pm **N. Marcella** *Machine Learning Analysis of XANES and EXAFS*
- 6:00pm Adjourn for dinner

Thursday, Nov 2

- 9:00am **A. Frenkel** *Overview of Athena and Artemis (Demeter data analysis package)*
- 10:00am **J. Timoshenko** *Software demonstration.*
Part 1: Wavelet transform analysis
- 10:30am Break
- 11:00am **J. Timoshenko** *Software demonstration.*
Part 2: Reverse Monte Carlo simulations and evolutionary algorithm
- 12:00pm **A. Kuzmin** *Software demonstration for Molecular Dynamics simulations of EXAFS spectra: Part 1*
- 1:00pm Adjourn for lunch
- 2:20pm **A. Kuzmin** *Software demonstration for Molecular Dynamics simulations of EXAFS spectra: Part 2*
- 3:20pm **K. Lomachenko** *Software demonstration for PCA and MCR-ALS.*
- 4:20pm Break
- 4:40pm **P. Routh** *Software demonstration for machine learning applications.*
- 6:00pm Adjourn for dinner

Friday, Nov. 3

9:00 Data analysis practicum

Instructors: J. Timoshenko, A. Kuzmin, K. Lomachenko, P. Routh, N. Marcella, R. Shimogawa, A. Frenkel

12:00pm Lunch

1:00pm Data analysis practicum

Instructors: J. Timoshenko, A. Kuzmin, K. Lomachenko, P. Routh, N. Marcella, R. Shimogawa, A. Frenkel

5:00pm Adjourn