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 + photo*

11:00am **A. Kuzmin** *The use of Molecular Dynamics simulations for the interpretation of EXAFS spectra*

12:00pm *Adjourn for lunch*

1:00pm J. **Timoshenko** *Obtaining 3D structure from EXAFS spectra. Part 1: Wavelet transform analysis*

1:30pm **J. Timoshenko** *Obtaining 3D structure from EXAFS spectra. Part 2: Reverse Monte Carlo simulations and evolutionary algorithm*

2:30pm **P. K. Routh** *Resolving spectral mixtures: linear combination fitting, principal component analysis and MCR-ALS*

3:30pm *Break*

4:00pm **N. Marcella** *Machine Learning Analysis of XANES and EXAFS*

5:00pm **Q & A***: Instructors and participants*

6:00pm *Adjourn for dinner*

Thursday, Nov 2

9:00am **A. Frenkel** *EXAFS data analysis and modeling of mono- and bimetallic nanoparticles (demonstration)*

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*

12:30pm *Adjourn for lunch*

1:30pm **A. Kuzmin** *Software demonstration for Molecular Dynamics simulations of EXAFS spectra: Part 2*

3:00pm **P. Routh** *Python for XAFS (Colab, plotting, etc.)*

3:30pm **P. Routh** *Software demonstration for PCA and MCR-ALS*

4:00pm *Break*

4:30pm **N. Marcella** *Software demonstration for machine learning applications.*

5:30pm **Q & A***: Instructors and participants*

6:00pm *Adjourn for dinner*

Friday, Nov. 3

9:00 Data analysis practicum

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

12:00pm *Break for Lunch*

1:00pm Data analysis practicum

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

Discussion for all groups

5:00pm *Adjourn*