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