

Short Course on X-ray Absorption Fine Structure: Theory, Data Analysis and Modeling Virtual Course

Agenda

Course Instructors: N. Marcella (UIUC/BNL), Y. Li (ORNL), A. Frenkel (SBU/BNL), S. Kelly (APS), F. Vila (UW), J. Kas (UW), P. Routh (SBU), H. Wang (SBU), J. Timoshenko (FHI), D. Sprouster (SBU), S. Xiang (SBU), J. Li (SBU), K. Zheng (SBU), L. Ma (NSLS-II)

Wednesday, Nov. 2

- 9:00 **A. Frenkel** *Welcoming remarks*
9:10 **A. Frenkel** *Introduction and overview of XAFS*
9:40 **N. Marcella** *EXAFS theory*
10:40 *Coffee break*
11:00 **J. Timoshenko** *Treatment of disorder in EXAFS analysis*
12:00pm *Lunch*
1:10pm **F. Vila** *Theory of XANES*
2:10pm **J. Kas** *FEFF9 code for XANES modeling*
3:10pm *Coffee break*
3:40pm **N. Marcella** *XAFS data processing with Athena and Larch (demo)*
4:30pm **D. Sprouster** *EXAFS data analysis by FEFF fitting*
5:10pm **Questions and Answers (participants and instructors)**
6:00pm Adjourn

Thursday, Nov. 3

- 8:30 *Breakfast*
9:00 **S. Kelly** *EXAFS data analysis with Artemis and Larch (demo)*
10:00 **J. Timoshenko** *Advanced topics: Multiple scattering EXAFS analysis*
11:00 *Coffee break*
11:20 **P. Routh** *XANES data analysis by Principal Component Analysis and MCR-ALS*
12:00pm *Lunch*
1:20pm **F. Vila** *FEFF9 code for XANES modeling (demo)*
2:20pm **N. Marcella** *Artificial neural network approach to XANES and EXAFS data analyses*
3:20pm *Coffee break*

3:40pm **A. Frenkel** *Structural analysis and modeling of mono- and bimetallic nanoparticles using EXAFS*
4:30pm **L. Ma** *In situ capabilities at the QAS beamline of NSLS-II*
5:00pm **Questions and Answers (participants and instructors)**
6:00pm Adjourn

Friday, Nov. 4

9:00 Data analysis practicum
Instructors: N. Marcella, Y. Li, A. Frenkel, S. Kelly, F. Vila, J. Kas, P. Routh, H. Wang, J. Li, D. Sprouster, S. Xiang, K. Zheng
12:00pm *Lunch*
1:00pm Data analysis practicum
Instructors: N. Marcella, Y. Li, A. Frenkel, S. Kelly, F. Vila, J. Kas, P. Routh, H. Wang, J. Li, D. Sprouster, S. Xiang, K. Zheng
5:00pm Adjourn