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

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**Friday, Nov. 4**

9:00  Data analysis practicum


12:00pm  *Lunch*

1:00pm  Data analysis practicum


5:00pm  Adjourn