

X-ray Absorption Fine Structure: Theory, Data Analysis and Modeling

Tentative Agenda (time slots may change)

Wednesday, November 13

Location: Medical Building 490, Large Seminar Room

8:30am Continental Breakfast (provided)
9:00am **Anatoly Frenkel** *Welcoming remarks*
9:10am **Anatoly Frenkel** *Introduction and overview of XAFS*
9:40am **John Rehr** *Theory of XANES*
10:40am Coffee Break (provided)
11:00am **Kirill Lomachenko** *EXAFS equation*
12:00pm Lunch (provided)
1:10pm **Anatoly Frenkel** *EXAFS data processing and analysis methods*
2:10pm **Erjia Guan** *XAFS data processing with Demeter/Athena (demo)*
3:10pm Coffee Break (provided)
3:40pm **Fernando Vila** *FEFF9 code for XANES modeling*
4:30pm **John Rehr** *Treatment of disorder in EXAFS analysis*
5:10pm **Kirill Lomachenko** *EXAFS data analysis by FEFF fitting*
6:00pm Dinner (provided) – Berkner Bldg. 488

Thursday, November 14

Location: Chemistry Building 555, Hamilton Seminar Room

8:30am Continental Breakfast (provided)
9:00am **Erjia Guan** *EXAFS data analysis with Demeter/Artemis (demo)*
10:00am **Fernando Vila** *FEFF9 code for XANES modeling (demo)*
11:00am Coffee Break (provided) and Group Photo
11:20am **Joseph Woicik** *Pre-edge features in XANES: application to materials research*
12:00pm Lunch (provided)
1:20pm **Anatoly Frenkel** *Advanced topics: Multiple scattering EXAFS analysis*
2:20pm **Kirill Lomachenko** *XANES data analysis by Principal Component Analysis and MCR-ALS*
3:20pm Coffee Break (provided)

- 3:40pm **Nicholas Marcella** *Artificial neural network approach to XANES and EXAFS data analyses*
- 4:40pm **Yuanyuan Li** *Structural analysis and modeling of mono- and bimetallic nanoparticles using EXAFS*
- 5:30pm **A. Frenkel** *Synchrotron Catalysis Consortium at BNL*
- 6:00pm *Dinner (provided) – NSLS-II Bldg. 743 (LOB3)*

Friday, November 15

Location: Berkner Building 488, Conference Room B

- 8:30am *Continental Breakfast (provided)*
- 9:00am Data analysis practicum
Instructors: K. Lomachenko, E. Guan, N. Marcella, Y. Li, A. Frenkel, F. Vila, J.Rehr
- 12:00pm *Lunch (provided)*
- 1:00pm Data analysis practicum
Instructors: K. Lomachenko, E. Guan, N. Marcella, Y. Li, A. Frenkel, F. Vila, J.Rehr
- 5:00pm *Adjourn*