

# 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 – be sure to pick up your meal tickets before proceeding to the cafeteria)*
- 1:10pm **Lu Ma** *XAFS 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) – NSLS-II building 743 (LOB 3)*

Thursday, November 14

Location: Medical Building 490, Large 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 – be sure to pick up your meal tickets before proceeding to the cafeteria)*
- 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 building 743 (LOB 3)*

**Friday, November 15**

Location: Medical Building 490, Large Seminar Room

- 8:30am *Continental Breakfast (provided)*
- 9:00am Data analysis practicum  
Instructors: A. Frenkel, E. Guan, J. Huang, J. Lee, Y. Li, K. Lomachenko, L. Ma, N. Marcella, N. Marinkovic, J.Rehr, Y. Tian, F. Vila, J. Woicik, Z. Xie
- 12:00pm *Lunch (provided – be sure to pick up your meal tickets before proceeding to the cafeteria)*
- 1:00pm Data analysis practicum  
Instructors: A. Frenkel, E. Guan, J. Huang, J. Lee, Y. Li, K. Lomachenko, L. Ma, N. Marcella, N. Marinkovic, J.Rehr, Y. Tian, F. Vila, J. Woicik, Z. Xie
- 5:00pm *Adjourn*