

Synchrotron Catalysis Consortium at BNL: In-Situ and Operando Experiments and Data Analysis

Nov. 6-8, 2024

Tentative Agenda (time slots may change)

Wednesday, Nov. 6

Session 1. Introduction to SCC

- 9:00am **A. Frenkel (SBU/BNL) and A. Harris (BNL)** *Welcoming remarks*
9:20am **J. G. Chen (Columbia/BNL)** *Synchrotron Catalysis Consortium (SCC)*
9:50am **A. Frenkel** *“Toolboxes” for probing structure-function relationships in catalysts*
10:30am Coffee Break + photo
11:00am **L. Miller (BNL)** *Overview of NSLS-II capabilities*
11:15am **J. Rodriguez (BNL)** *New approaches for the trapping and conversion of CO₂: Synchrotron - based studies*
12:00pm Adjourn for lunch

Session 2. Methods

- 1:00pm **Z. Xie (Columbia)** *In situ/operando X-ray absorption spectroscopy*
1:30pm **N. Marinkovic (Columbia)** *In situ/operando infrared spectroscopy*
2:00pm **J. Yang (CFN/BNL)** *In situ/operando electron microscopy*
3:00pm Break
3:30pm **S. Ghose (NSLS-II/BNL)** *In situ/operando X-ray diffraction*
4:15pm **A. Frenkel** *Problem-solving methods using XANES and EXAFS*
5:00pm **Q & A: Instructors and participants**
6:00pm Adjourn for dinner

Thursday, Nov. 7

Session 3. Tutorials

- 9:00am **A. Frenkel** *EXAFS data analysis and modeling of nanocatalysts*
10:00am **K. Lomachenko (ESRF)** *Speciation of heterogeneous mixtures by principal component analysis and MCR ALS*
11:00am Coffee Break
11:30am **A. Frenkel** *EXAFS data analysis and modeling of mono- and bimetallic nanoparticles (demonstration)*
12:15pm **K. Lomachenko** *Speciation of heterogeneous mixtures by principal component analysis and MCR ALS (demonstration)*

1:00pm Adjourn for lunch

Session 4. Quo vadis?

2:00pm **N. Marinkovic** *Electrocatalysis experiments (perspective)*

2:30pm **J. Rodriguez** *High pressure experiments (perspective)*

3:00pm **M. Nachtegaal (PSI)** *Modulation excitation spectroscopy experiments*

3:30pm Break

4:00pm **A. Frenkel** *New directions in data analysis employing machine learning*

4:30pm **L. Miller (NSLS-II/BNL)** *Guidance for general user proposal preparation*

5:00pm **Q & A: Instructors and participants**

6:00pm Adjourn for dinner

Friday, Nov. 8

9:00 Data analysis practicum

Instructors: Z. Xie, N. Marinkovic, K. Zheng, S. Xiang, K. Lomachenko, M. Nachtegaal,
A. Frenkel

12:00pm Adjourn for Lunch

1:00pm Data analysis practicum

Instructors: Z. Xie, N. Marinkovic, K. Zheng, S. Xiang, K. Lomachenko, M. Nachtegaal,
A. Frenkel

Discussion for all groups

5:00pm Adjourn