

# 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)** *Welcoming remarks*
- 9:20am **J. G. Chen (Columbia/BNL)** *Synchrotron Catalysis Consortium (SCC)*
- 9:50am **J. Rodriguez (BNL)** *New approaches for the trapping and conversion of CO<sub>2</sub>: Synchrotron - based studies*
- 10:30am *Break + photo*
- 11:00am **A. Frenkel** *“Toolboxes” for probing structure-function relationships in catalysts*
- 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 *Examples from multimodal/operando research*
- 4:15pm *Practical session*
- 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 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 **A. Frenkel** *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, Lomachenko, Nachtegaal, A. Frenkel

12:00pm Adjourn for Lunch

1:00pm Data analysis practicum

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

Discussion for all groups

5:00pm Adjourn