SUNCAT Summer Institute Program

Day 1: Aug 7, 2023

Morning Session

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor), Stanford Campus

12:00-13:00: Check-in for attendees

Afternoon Session

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Adam S. Hoffman

13:15-14:00: Welcome and Announcements

Tom Jaramillo Frank Abild-Pederson

14:00-14:15: Questions + Break

14:15-15:00: Yang Shao-Horn

Catalyzing Net-Zero [Placeholder]

15:00-15:15: Questions + Break

15:15-16:00: Tejs Vegge

Uncertainty-aware ML-models for catalytic solid-liquid interfaces and reaction

networks

16:00-16:15: Questions + Break

16:15-17:00: Aditya Bhan

Concepts relevant for the kinetic analysis of reversible reaction systems

Evening Session

Location: Shriram Center Tea Room & Sunken Terrace, Stanford Campus

17:00-18:30: Poster Session 1

Day 2: Aug 8, 2023

Morning Session

Location: Shriram Center, Stanford Campus

8:00-8:20: Grab-and-Go Breakfast

Location: Hewlett 200, Stanford Campus **Session Chair:** Michaela Burke Stevens

8:30-9:15: Yuriy Román

9:15-9:30: Questions + Break

9:30-10:15: Steven Torrisi

Representations Across Length Scales in Materials Science

10:15-10:30: Questions + Break

10:30-11:15: Panel Discussion: Careers In Catalysis

Moderator:

Simon R. Bare

Panelists:

Steven Torissi Aditya Bhan Adam Nielander

11:15-11:30: Questions + Break

11:30-12:15: Anastassia Alexandrova

Interfacial fluxionality in electrocatalysis: the ever-changing nature of the active

site

Lunch (12:15-13:15)

Location: Shriram Center, Stanford Campus

Afternoon Session

Location: Hewlett 200, Stanford Campus

Session Chair: Adam Nielander

13:15-14:00: Jesus Valazquez

Unraveling CO2 and CO Conversion to Alcohols in Multinary Metal

Chalcogenides

14:00-14:15: Questions + Break

14:15-15:00: Linsey Seitz

Characterizing Dynamic Materials for Sustainable Electrocatalytic Technologies

15:00-15:15: Questions + Break

15:15-16:00: Heather Kulik

Addressing challenges for electronic structure and machine learning in open shell

transition metal catalysis

16:00-16:15: Questions + Break

16:15-17:00: Networking Time

Evening Session

Location: Shriram Center Tea Room & Sunken Terrace, Stanford Campus

17:00-18:30: Poster Session 2

Day 3: Aug 9, 2023

Morning Session

Location: Shriram Center, Stanford Campus

8:00-8:20: Grab-and-Go Breakfast

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Kirsten Winther

8:30-9:15: Ib Chorkendorff

The Challenge of Activating Nitrogen

9:15-9:30: Questions + Break

9:30-10:15: Alper Uzun

Tuning catalytic performance and stability of atomically dispersed supported

metal catalysts

10:15-10:30: Questions + Break

10:30-11:15: Panel Discussion: DEI In Catalysis

Moderator:

Tom Jaramillo

Panelists:

Susannah Scott Linsey Seitz Jesus Velazguez

11:15-11:30: Questions + Break

11:30-12:15: Paul Dauenhauer

Fundamental Concepts in Programmable Surface Chemistry

Lunch & Photo (12:15-13:15)

Location: Shriram Center, Stanford Campus

Photo Location TBD

Afternoon Session

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Daniel Lee

13:15-14:00: Ismaila Dabo

Data-Informed Discovery of Earth-Abundant Photocatalysts for Hydrogen

Generation

14:00-14:15: Questions + Break

14:15-15:00: SUNCAT Session - Michal Bajdich & Kirsten Winther

Computational tools for catalysis and data sharing: hands-on tutorial in Python

15:00-15:15: Questions + Break

15:15-16:00: Susannah Scott

Connecting X-ray spectroscopy to kinetics to understand Ga-based dehydrogenation catalysts

16:00-16:15: Questions + Break

16:15-17:00: Jeremy Feaster

Building the Next Generation of Electrochemical Reactors through Advanced Manufacturing

Evening Session

Location: Manzanita Field, Stanford Campus

17:00-18:30: Beach Volleyball

Day 4: Aug 10, 2023

Morning Session

Location: Shriram Center, Stanford Campus

8:00-8:20: Grab-and-Go Breakfast

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Michal Bajdich

8:30-9:15: Charlotte Vogt

The Concept of Active Site in Catalysis

9:15-9:30: Questions + Break

9:30-10:15: Liane Rossi

Metal-ligand cooperation in heterogeneous catalysis

10:15-10:30: Questions + Break

10:30-11:15: Panel Discussion: Future of Sustainable Catalysis

Moderator:

Frank Abild-Pederson

Panelists:

Tejs Vegge

Paul Dauenhauer Olga Safonova Charlotte Vogt

11:15-11:30: Questions + Break

11:30-12:15: Olga Safonova

Design of XAS experiments for uncovering active sites in heterogeneous

catalysts

<u>Lunch</u> (12:15-13:15)

Location: Shriram Center, Stanford Campus

Afternoon Session

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Johannes Voss

13:15-14:00: Karsten Reuter

Data-enhanced multiscale modeling of heterogeneous catalysis

14:00-14:15: Questions + Break

14:15-15:00: SUNCAT Session - Adam Hoffman

Operando Catalysis Experiments using X-ray Absorption Spectroscopy

15:00-15:15: Questions + Break

15:15-16:00: Networking Time

16:00-16:15: Questions + Break

Evening Session

Location: Chuck Taylor Grove, Stanford Campus

16:15-18:30: BBQ & Poster Awards

Day 5: Aug 11, 2023

Morning Session

Location: Shriram Center, Stanford Campus

8:00-8:20: Breakfast

Location: Li Ka Shing Learning and Knowledge Center (Paul & Mildred Berg Hall, 2nd floor),

Stanford Campus

Session Chair: Matteo Cargnello

8:30-9:15: Poster Award Winner Talks 1-3 (10 min talk + 5 min questions)

1. Ankita Kumari

2. Tana Siboonruang

3. Davide Menga

9:15-9:30: Break

9:30-10:15: Poster Award Winner Talks 4-6 (10 min talk + 5 min questions)

4. Anukriti Shrestha

5. Rachita Rana

6. Aniket Mule & Yamile Cornejo-Carrillo

10:15-10:30: Closing Remarks - Tom Jaramillo

10:45-13:00: SLAC Tour [Participants Emailed]

Grab and Go Lunch