

## FUNCAT / Center2Center Symposium (12<sup>th</sup>-14<sup>th</sup> of April 2022)

### April 12 (Tuesday):

Arrival and check in at the Harnack-House

### April 13 (Wednesday):

**09:00-09.05** Opening / Welcome (F. Schüth, G. Hutchings)

**09:05-10:00** *Plenary Lecture 1*, Ferdi Schüth, *Mechano-chemical synthesis and catalysis*

**10:00-10:30** Eylül Öztuna, *Pd thin film catalysts for acetylene hydrogenation*

**10:30-11:00** *Coffee-Break*

**11:00-11:30** Sam Pattison, *Au/C catalysts for acetylene hydrochlorination: an overview of recent progress and future challenges*; Jake Williams, *Investigating the difference between gas and liquid phase alkyne hydrogenation*

**11:30-12:00** Klara Sophia Kley & Jacopo de Bellis, *Selective hydrogenation of highly concentrated acetylene streams over mechanochemically-synthesized PdAg supported catalysts*

**12:00-12:30** Mark Douthwaite, *Cooperative redox enhancement effects in bimetallic catalysis*

**12:30-13.30** **Lunch-Break**

**13.30-14:30** *Plenary Lecture 2*, Graham Hutchings, *Au nanoparticle and alloys for oxidation reactions*

**14.30-15:00** Kendra Belthle, *Cobalt-support interaction effects in CO<sub>2</sub> hydrogenation*

**15:00-15:30** **Coffee-Break**

**15:30-16:30** **Flash presentations** (3 minutes short presentations, the program is given below)

**16:30- 18:30** **Poster session / further group discussions**

**19:00-22:00** **Symposium Dinner**

## **April 14 (Thursday):**

**09:00-10:00** *Plenary Lecture 3, Annette Trunschke, Re-thinking experimental approaches in catalysis research: why artificial intelligence-assisted discovery of new catalysts will benefit from rigorous experimental protocols and automation*

**10:00-10:30** *Lucas Foppa, Identifying the materials genes of selective oxidation with clean experiments and artificial intelligence*

**10:30-11:00** *Coffee-Break*

**11:00-11:30** *David Willock & Herzain Rivera, Hydrogen adsorption on Pd surfaces and its effect on CO<sub>2</sub> Activation*

**11:30-12:00** *Igor Kowalec, Cu, Pd and Zn surfaces for CO<sub>2</sub> activation and hydrogenation*

**12:00- 12:15** **Final remarks & closing symposium**

**12:15** **Lunch & Departure**

## *Flash Presentations*

### *Acetylene Chemistry*

1. **Anna Lazaridou:** Sulfur promotion in Au/C catalyzed acetylene hydrochlorination
2. **Yanlin Wang:** Active sites of Pt-based catalysts in acetylene hydrochlorination reaction
3. **Özgül Agbaba:** Oligomerization of acetylene to 1,3-butadiene

### *CO<sub>2</sub> Reduction*

4. **Tugce Beyazay:** Hydrothermal CO<sub>2</sub> reduction over Ni-Fe nanoparticles
5. **Ray Miyazaki:** AI with experimental and theoretical data: role of the support material for CO<sub>2</sub> hydrogenation
6. **Isla E. Gow:** The effect of support surface area on Pd/ZnO catalysts for CO<sub>2</sub> hydrogenation to methanol.
7. **Naomi Lawes:** Investigating the formation of active PdZn nanoparticles for CO<sub>2</sub> hydrogenation to methanol

### *Selective Oxidation*

8. **Fenglou Ni:** Aqueous Au-Pd colloids catalyze selective methane oxidation to methanol with oxygen under mild conditions
9. **Isaac T. Daniel:** Au-Pd separation enhances bimetallic catalysis of alcohol oxidation
10. **Joseph Brehm:** Chemo-enzymatic cascades poptimising selective C-H Oxidation
11. **Kai Wang:** The promotional effect of calcination treatment on Pd/C catalyst for solvent-free benzyl alcohol oxidation

### *H<sub>2</sub>O<sub>2</sub> Generation*

12. **Alexander STENNER:** A chemo-enzymatic oxidation cascade to activate C-H bonds with in-situ generated H<sub>2</sub>O<sub>2</sub>
13. **Ashley Ward:** The ffect of pre-treatment of the support for the direct synthesis of H<sub>2</sub>O<sub>2</sub>
14. **Greg Sharp:** Enhanced selective oxidation of benzyl alcohol via in situ H<sub>2</sub>O<sub>2</sub> production over supported Pd-Based catalysts
15. **Ben Bayntun:** Utilisation of in situ generated H<sub>2</sub>O<sub>2</sub> for greywater remediation

### *Synthesis and Beyond*

16. **Rohini Khobragade:** Catalysts synthesis via mechanochemical method
17. **Sofia Mediavilla Madrigal:** Characterisation of novel trimetallic catalysts for CO Activation
18. **Bolun Wang:** Bipyridine embedded polyphenylene porous organic polymers for anchoring Au and Cu Single Sites