CRC 1625

Agenda Retreat

07. – 09.10.2024

07.10.2024 Monday	
11:45	**Arrival**
12:00 – 13:00	**Lunch**
Presentation and discussion session of Area A (Short summary, newest results, next steps – (time: presentation + discussion))	
13:00 – 13:30	**Overview CRC1625** Alfred Ludwig (20 + 10)
13:30 – 13:45	**Overview Research Area A** Alfred Ludwig (10 + 5)
13:45 – 14:10	**A01** Christian Møgelberg Clausen and Natalia Pukhareva (10 + 15)
14:10 – 14:35	**A02** Rico Zehl (10 + 15)
14:35 – 16:00	**Break** (check-in to rooms, then coffee and snacks available)
16:00 – 16:25	**A03** Ralf Drautz (10 + 15)
16:25 – 16:50	**A04** Jörg Neugebauer (10 + 15)
16:50 – 17:15	**A05** Markus Stricker (10 + 15)
17:15 – 17:40	**A06** Samuel García (10 + 15)
17:40 – 18:30	**Break**
18:30 – 19:30	**Dinner**
19:30 - open	**Evening program (networking)**

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08.10.2024 Tuesday (01)	
07:30 – 09:00	**Breakfast**
08:30 – 09:00	**Walking around the castle (if you want)**
Presentation and discussion session of Area B (Short summery, newest results, next steps – (time: presentation + discussion))	
09:00 – 09:15	**Overview Research Area B** Tina Scheu (10 + 5)
09:15 – 09:40	**B01** Yujiao Li (10 + 15)
09:40 – 10:05	**B02** Tong Li (10 + 15)
10:05 – 10:30	**B03** Christoph Somsen (10 + 15)
10:30 – 10:50	**Break** (Coffee and snacks available)
10:50 – 11:15	**B04** Baptiste Gault (10 + 15)
11:15 – 11:40	**B05** Karina Morgenstern (10 + 15)
11:30 – 13:00	**Break** and **Lunch** at 12:00
Presentation and discussion session of Area C (Short summary, newest results, next steps – (time: presentation + discussion))	
13:00 – 13:15	**Overview Research Area C** Corina Andronescu (10 + 5)
13:15 – 13:40	**C01** Wolfgang Schuhmann (10 + 15)
13:40 – 14:05	**C02** Corina Andronescu (10 + 15)
14:05 – 14:30	**Break** (Coffee and snacks available)
14:30 – 14:55	**C03** Kristina Tschulik (10 + 15)
14:55 – 15:20	**C04** Aliaksandr Bandarenka (10 + 15)

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08.10.2024 Tuesday (02)	
15:30 – 16:45	**Afternoon Group Activity (Walk ~1:15 h to distillery *Kornbrennerei Böckenhoff*)**
16:45 – 18:00	**Visit distillery *Kornbrennerei Böckenhoff***
18:00 – 20:15	**Walk back or by public bus 18:37 or 19:37 [Erle, Silvesterstraße]), Break**
20:15 – 21:45	**Dinner**

09.10.2024 Wednesday	
07:30 – 09:00	**Breakfast**
08:30 – 09:00	**Walking around the castle (if you want)**
Presentation and discussion session of Service and General Projects (Short summary, practical sessions, next steps – (time: presentation + discussion))	
09:00 – 09:40	**INF and Research Data Management with hands-on session (examples, problem solving)** Markus Stricker/Victor Dudarev (20 + 20)
09:40 – 10:00	**Project S** Janine Pfetzing (10 + 10)
10:00 – 10:20	**Project Z** Sabrina Baha (10 + 10)
10:20 – 10:45	**RTG (election)** Tong Li/Wolfgang Schuhmann (10 + 15)
10:45 – 11:00	**Break** (Coffee and snacks available)
Synergistic methods **(Parallel) working session (see additional information)**	
11:00 – 13:00	**Block A (lead: A01)** **Block B: (lead: B03)** **Block C (lead: A05/A06)**
13:00 – 14:00	**Lunch**
14:00 – 14:30	**SAA representations (A03)** Ralf Drautz (10 + 20)
14:30 – 15:00	**Identification of SAA by combining simulation and experiments (C01)** Wolfgang Schuhmann (10 + 20)

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Organization Parallel working	
15:00 – 16:00	**Interactions between CRC members, second RDMS hands-on session**
15:00 – 16:00	**Steering Board** With steering board members
15:00 – 16:00	**Organization for Early Career Retreat** With early career researchers and RTG, project Z
16:00	**Departure**

Synergistic methods:

Block A

A01, A02, A03, A04, B01, C01, S

Material platform (A01) (p. 55)

- **Materials Selection:** What are the next CCSS systems for catalytic and surface analysis?
- **Methodology and Characterization:** How successful is our loop experiment ←→ modelling?
- **Collaborative Research:** sample storage, and feedback for material optimization.

Block B

B02, B03, B04, C02, C03, C04

Holistic characterisation (B03) (p. 57)

- **Synergistic Methods**: Challenge in integrating diverse characterization techniques. How can we ensure the data from each method remains coherent when combined?
- **Electrochemical Activity Correlation**: How can we improve the correlation between experimental electrochemical measurements and theoretical predictions

Block C

A05, A06, RDM, INF

- **Combining Simulation and Experimental Data**: How can we optimize the integration of simulation and experimental datasets to ensure more accurate predictions of SAA properties?
- **Data Fusion**: What strategies should we adopt to ensure that machine learning models are robust and provide accurate predictions?
- **Developing a Standardized Ontology for SAA**: How do we ensure that the ontology captures all relevant aspects of SAA while remaining flexible enough to accommodate future discoveries?
- **Digital Tools**: What features should our digital platform include to best support real-time collaboration?

Together

1. SAA representations (A03) (p. 62)

- **SAA Representations**: What are the advanced and flexible representations of SAA, suitable for computational analysis? What are the advantages and limitations of the different SAA representation methods (e.g., cluster expansion, ACSF, SOAP)?
- **Variations in Surface Structures**: How do we best account for surface defects and irregularities in SAA representations?
- **Linking SAA Representations to Electrocatalytic Properties**: How can we improve the link between atomic-scale SAA representations and measurable catalytic properties? What strategies should we use to reduce the complexity of these representations without losing critical information?

2. Identification of SAA by combining simulations and experiments (C01)

- **Synergistic Use of Experimental and Simulation Techniques**: How can we best combine experimental and simulation techniques to gain a comprehensive atomic-scale understanding of SAA? What challenges do we face in integrating results from diverse methods?
- **Proxy and Simulation Support**: What role do proxy measurements play in SAA identification? How can we ensure the accuracy and reliability of such measurements in predicting real surface compositions?
- **Feedback Loop**: How can we create an efficient feedback loop between simulations and experiments? What strategies can be used to resolve discrepancies between predicted and observed SAA structures?