



CRC 1109



# CRC WORKSHOP

## Edith Flanigen Award 2014

9.-10. October 2014

Erwin Schrödinger-Zentrum Adlershof  
Rudower Chaussee 26  
12489 Berlin  
room 0'119

contact:

CRC 1109 office  
phone +49 30 2093-66118  
email: sfb1109@hu-berlin.de

<https://www.chemie.hu-berlin.de/sfb1109/>

### — October 9<sup>th</sup> (Thursday) —

09.00 project presentations I

**chair: Thomas Braun**

project **A01** (Thomas Braun) 09:00

- Oxygenation of subvalent aluminum compounds: reactions of oxo compounds with water and silanols to access aluminosiloxanes — *Adrian Stelzer (HU)*
- From subvalent silicon compounds to siloxanes by oxygenation, hydrolysis and condensation — *Philipp Roesch (HU)*

project **A02** (Franziska Emmerling/Ralph Krähnert) 09:40

- Characterization of nucleation, growth, and crystallization of iron oxide nanoparticles — *Anke Kabelitz (BAM)*
- Crystallization and dissolution of nanoscaled iron oxides — *Katrin Schulz (TU)*

project **A03** (Martin Kaupp) 10:20

- Reactions of small oxo clusters in aqueous environments. A quantum-chemical perspective — *Robert Müller (TU)*

10.40 coffee break

11.10 project presentations II

project **A03** (Martin Kaupp) 11:10

- Dealing with aqueous environments in quantum-chemical calculations — *Martin Enke (TU)*

project **A04** (Christian Limberg) 11:30

- Targeted construction and reactivities of novel, molecular Si-O-Al model compounds — *Kapil Lokare (HU)*
- Molecular iron silicates: Well-defined small oxo aggregates — *Nicole Manicke (HU)*

project **A05** (Christoph Schalley) 12:10

- Studying solution and gas phase chemistry of oxido clusters by mass spectrometry — *Ulrike Warzok (FU)*

12.30 lunch

14.10 project presentations III

project **A06** (Bernd Jürgen Winter) 14:10

- Electronic structure of square-planar high-spin Fe(II) O<sub>4</sub> in aqueous solution studied by liquid-jet X-ray spectroscopies — *Robert Seidel (HZB)*

related lecture: 14:30

- Ab initio investigation of the water/MgO(001) interface — *Milan Oncak (HU)*

**chair: Kramer Campen**

project **B01** (Kramer Campen/Peter Saalfrank) 14:50

- Understanding the interaction of water and alpha-alumina: Experiment and theory — *Jonas Wirth (UP), Harald Kirsch (FHI)*

project **B02** (Hans-Joachim Freund/S. Shaikhutdinov) 15:30

- Interaction of water with silica and aluminosilicate thin films — *Emre Emmez (FHI)*
- Surface science approach toward understanding oxide supported catalysts in contact with water — *Yuichi Fujimori (FHI)*

project **B03** (Eckard Rühl) 16:10

- Mechanisms of nucleation and growth of oxide nanoparticles studied by single, levitated microparticles — *René Dallinger (FU)*

16.30 coffee break + PI meeting

17.15 evening lecture

**Luisa de Cola**, Université de Strasbourg  
Hybrid porous materials. Properties and applications

— October 10<sup>th</sup> (Friday) —

09.00 project presentations IV

chair: Erhard Kemnitz

project **C01** (Erhard Kemnitz/Gudrun Scholz) 09:00

- Introduction of structural distortion by bottom up methods: Amorphous fluoride-doped aluminum Oxides and hydroxides and new crystalline model-clusters — *Lukas Ahrem (HU)*
- Mechanochemical synthesis and activation of New Low-fluorine doped aluminium oxides and iron (III)-oxides — *Valentina Scalise (HU)*

project **C02** (Elena Voloshina/Joachim Paier) 09:40

- Effect of the environment on  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>(0001) surface structures — *Roman Ovcharenko (HU)*
- Adsorption of water on the Fe<sub>3</sub>O<sub>4</sub>(111) surface: A DFT+U study — *Joachim Paier (HU)*

project **C03** (Beate Paulus) 10:20

- Theoretical investigations for aluminium-alkoxide fluoride clusters including solvent effects — *Johannes Budau (FU)*

10.40 coffee break

11.10 project presentations V

project **C04** (Nicola Pinna) 11:10

- Oxide nanostructures: growth and surface reactivity studied at mbar pressure by atomic layer deposition — *Guylhaine Clavel (HU)*

project **C05** (Thomas Risse) 11:30

- Reactivity of point defects on single crystalline silica and aluminosilicate surfaces with water — *Nina Richter (FU)*

chair: Joachim Sauer

project **D01** (Knut Asmis) 11:50

- Gas phase vibrational spectroscopy of mass-selected aluminum oxide anions — *Xiaowei Song (FHI)*
- Structure characterization of metal oxide clusters in the gas phase: Experimental setup and technique — *Matias Fagiani (FHI)*

12.30 lunch

14.10 project presentations IV

project **D02** (Joachim Sauer/Florian Bischoff) 14:10

- The geometric and electronic structure of small aluminum oxide clusters — *Florian Bischoff (HU)*

project **D03** (Matthias Drieß) 14:30

- Non-hydrolytic pathways to silica and its analogues and molecular models of silica surfaces with oxygen defects and Si=O groups — *Gengwen Tan (TU), Yun Xiong (TU)*

project **D04** (Joachim Sauer) 15:10

- Hydration and hydrolysis in the dealumination and desilication of zeolites — *Itzar Goikoetxea (HU)*

concluding remarks

15.30 coffee break

**16.00 Edith Flanigen Award 2014**

**Awardee 2014:**

**Natacha Krins**

Laboratoire de Chimie de la Matière Condensée de Paris / Collège de France

opening remarks

speech by Edith Flanigen

laudation by Christian Limberg

bestowal of the Edith Flanigen Award

lecture by the awardee

reception