

# Programme

## Sunday, February 19, 2017

17:00	— Arrival —
18:00-19:30	— Dinner —
19:30-22:00	<b>Poster Session I</b>

## Monday, February 20, 2017

09:15-09:30	<b>Welcoming</b>	page
	<b>Session 1</b> (Chairman: <i>Ralph Krähnert</i> , Berlin, Germany)	
09:30-10:15	<b>Michael Fröba</b> (Hamburg, Germany) Phase behavior of confined water in ordered nanoporous organosilica hybrid materials with periodically modulated surface polarities	1
10:15-10:45	<b>R. Kramer Campen</b> (Berlin, Germany) How Metal Oxides Structure Interfacial Liquid Water: the Curious Case of the $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001)/Liquid Water Interface	2
10:45-11:15	— Coffee —	
	<b>Session 2</b> (Chairman: <i>Beate Paulus</i> , Berlin, Germany)	
11:15-12:00	<b>Christophe Copéret</b> (Zürich, Switzerland) Consequence of Water Adsorption and Hydroxylation Level on the Reactivity of Oxide Surfaces	3
12:00-12:30	<b>Joachim Sauer</b> (Berlin, Germany) Hydroxyl groups on metal oxide surfaces and clusters	4
12:30-13:00	<b>Céline Chizallet</b> (Solaize, France) Surface acidity of alumino-silicates: the key-role of the water/oxide interface	5
13:00-14:30	— Lunch —	

<b>Session 3</b> (Chairman: <i>Shamil Shaikhutdinov</i> , Berlin, Germany)		
14:30-15:15	<b>Helmut Cölfen</b> (Konstanz, Germany) Investigation of Prenucleation clusters, Nucleation and early growth species by Analytical Ultracentrifugation	6
15:15-15:45	<b>Franziska Emmerling</b> (Berlin, Germany) In-situ characterization of nucleation, growth, crystallization and dissolution of nanoscaled iron oxides	7
15:45-16:15	— Coffee —	
<b>Session 4</b> (Chairman: <i>Gudrun Scholz</i> , Berlin, Germany)		
16:15-17:00	<b>Angelos Michaelides</b> (London, UK) What we do and don't know about water at interfaces – molecular level insight from computer simulation	8
17:00-17:30	<b>Knut R. Asmis</b> (Leipzig, Germany) Structure of Bare and Microhydrated Aluminum Oxide Clusters in the Gas Phase	9
17:30-18:00	<b>Natacha Krins</b> (Paris, France) Mesoporous semiconducting oxides for Li-ion batteries: a light-assisted recharge	10
18:00-19:30	— Dinner —	
19:30-22:00	<b>Poster Session II</b>	

## Tuesday, February 21, 2017

<b>Session 5</b> (Chairman: <i>Kallol Ray</i> , Berlin, Germany)		<i>page</i>
09:00-09:45	<b>T. Don Tilley</b> (Berkeley, USA) Highly Oxidized Centers in Metal Oxides for Water Splitting	11
09:45-10:15	<b>Hans-Joachim Freund</b> (Berlin, Germany) Iron oxide, silica and modified silica and its interaction with water	12
10:15-10:45	— Coffee —	
<b>Session 6</b> (Chairman: <i>Thomas Braun</i> , Berlin, Germany)		
10:45-11:30	<b>Lee Cronin</b> (Glasgow, UK) Consequence of Water Adsorption and Hydroxylation Level on the Reactivity of Oxide Surfaces	13
11:30-12:00	<b>Matthias Drieß</b> (Berlin, Germany) Low-molecular weight models of silica and its heavy analogues: synthesis of isolable monomeric silanoic acid and silicon dichalcogenide compounds	14
12:00-12:30	<b>Martin Kaupp</b> (Berlin, Germany) Small Silicon and Aluminum Oxo Clusters. Benchmark Studies, Electronic Structure, Spectroscopy, and Reactivity	15
12:30-14:30	— Lunch —	

<b>Session 7</b> (Chairman: <i>Erhard Kemnitz</i> , Berlin, Germany)		
14:30-15:15	<b>Yves Chabal</b> (Dallas, USA) Chemistry in Confined Environments: Water Reaction in MOF-74	16
15:15-15:45	<b>Nicola Pinna</b> (Berlin, Germany) Metal Oxide Nanostructures Grown by Atomic Layer Deposition	17
15:45-16:15	— Coffee —	
<b>Session 8</b> (Chairman: <i>Liane G. Benning</i> , Potsdam, Germany)		
16:15-17:00	<b>William H. Casey</b> (Davis, USA) Pathways for oxygen-isotope exchange and dissociation in sets of oxide nanoclusters and minerals	18
17:00-17:30	<b>Christian Limberg</b> (Berlin, Germany) Aluminium and iron oxide/hydroxide clusters and frameworks in molecular compounds – Early stage modelling, tailored structural motifs and water reactivity	19
17:30-18:00	PI Meeting	
18:00-19:30	— Dinner —	
19:30-22:00	<b>Poster Session III</b>	

### Wednesday, February 22, 2017

<b>Session 9</b> (Chairman: <i>Peter Saalfrank</i> , Potsdam, Germany) <span style="float: right;"><i>page</i></span>		
09:00-09:45	<b>Michiel Sprik</b> (Cambridge, UK) All-atom DFT simulation of charged metaloxide-electrolyte interfaces	20
09:45-10:15	<b>Joachim Paier</b> (Berlin, Germany) Water interaction with iron oxides	21
10:15-10:45	— Coffee —	
<b>Session 10</b> (Chairman: <i>Robert Seidel</i> , Berlin, Germany)		
10:45-11:30	<b>Kevin Rosso</b> (Washington, USA) Understanding Electron Transfer Across Iron Oxide/Water Interfaces	22
11:30-12:00	<b>Bernd Winter</b> (Berlin, Germany) Aqueous phase metal-oxide nanoparticles and their early formation stages explored by liquid-jet soft-X-ray photoemission	23
12:00-12:30	<b>General discussion</b>	
12:30-14:30	— Lunch & Departure —	

## Poster presentations

(All posters will be presented every evening.)

A01	Hydrolysis and Condensation on a Ring-Strained Molecular Siloxandiol	P1
A01	Al and Al-Siloxaneclusters as Model Systems for Condensation and Hydrolysis reactions	P2
A02	First synthesis of magnetic monometallic iron oxide films with ordered mesopore structure	P3
A02	Understanding the crystallization of mesoporous iron oxide films: mechanism, kinetics and stabilization of the pore system	P4
A02	Time-resolved WAXS studies on the crystallization of Al <sub>13</sub> keggin clusters	P5
A03	Quantum Chemical Studies of Silicon Oxo/Hydroxo Systems in Aqueous Solution	P6
A04	Targeted Construction and Reactivities of Novel Molecular Si–O–Al Model Compounds	P7
A04	Iron Silsesquioxanes as Molecular Models for Iron Silicates	P8
A05	Probing Solution and Gas-phase Reactivity of Silicon-Oxo and Metal-Oxo Complexes by Means of Mass Spectrometry	P9
A06	Electronic structure of small iron oxide molecular frameworks and their precursors in aqueous solution	P10
B01	Water dissociative Adsorption on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (11 $\bar{2}$ 0)	P11
B01	Probing Surface Reconstruction of $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (11 $\bar{2}$ 0) Induced by Water Adsorption using Optical Surface Phonon Spectroscopy	P12
B01	Vibrational dynamics of H <sub>2</sub> O on hydroxylated $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001) surface: insights from simulations and VSF experiments	P13
B02	Characterization of Silica Surfaces with Scanning Probe Microscopy – Thin Films vs. Bulk	P14
B02	TPD study of H <sub>2</sub> O and CO <sub>2</sub> adsorption on (001) and (111) surfaces of Fe <sub>3</sub> O <sub>4</sub>	P15
B03	Investigation of iron and silicon oxide formation in single levitated micro droplets by Raman and X-Ray fluorescence spectroscopy	P16

C01	Al <sup>IV</sup> - and Al <sup>V</sup> -sites in Fluoride-doped Aluminum (hydr)oxides	P17
C01	Mechanochemical synthesis of low-fluorine doped aluminium (hydr)oxide fluorides	P18
C02	Heat of adsorption of water on the Fe <sub>3</sub> O <sub>4</sub> (111) surface studied by density functional theory	P19
C02	The crystal and electronic structure effects on water adsorption on hematite (0001) at various environment conditions	P20
C03	First-principle investigations of water adsorption on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> surfaces: The influence of fluoride defects	P21
C03	First-principle investigations of aluminiumoxofluoride clusters and their interaction with water	P22
C04	Single step transformation of CNTs to SiO <sub>2</sub> nanotubes via an atomic layer deposition process	P23
C05	Hydroxylation of thin silica film supported on Ru(0001) investigated by High Resolution Electron Energy Loss Spectroscopy	P24
D01	Vibrational Spectroscopy of Water Adsorption on Metal Oxide Clusters	P25
D01	Mass Spectrometry and Vibrational Spectroscopy of Silicate and Fe-Hydroxyl Oligomers	P26
D03	Synthesis and reactivity of silicon suboxides as molecular models of silica surfaces	P27
	Formation of molecular Iron-Oxide Clusters and their water reactivity studies	P28
	Local quantum chemical methods applied to adsorption: (i) water on SiO <sub>2</sub> , (ii) inter-layer interaction in black phosphorus	P29
	Ab initio simulation of of the external surface of zeolite Beta	P30