33.Workshop: Novel Materials and Superconductivity

Monday, 12.Feb. Chair: Günther Rupprechter

14.00 G. **Rupprechter** (TU Wien): *Opening, 33rd WS*

14:10 Thomas **Bürgi** (Uni Geneva):
On the Reactivity of Monolayer-Protected Metal Clusters

15:10 Short **Break**

15:30 Gerhard **Mestl** (Clariant):
High-Throughput Optimization of Catalytic Materials

16:30 **Coffee Break**

17:00 Alexey **Cherevan** (TU Wien):
State-of-the-art, Challenges and Prospects of Photocatalysis

Evening session **Chair: Ulrike Diebold**

19:30 Julia **Kunze-Liebhäuser** (Uni Innsbruck):
Electro-Activation of Small Molecules at the Solid/Liquid Interface

20:00 Iwona **Rutkowska** (Uni Warsaw):
Mixed-Metal Oxide Supports for Efficient Electrocatalysis

Thursday, 15.Feb. Chair: Bertram Batlogg

14:00 Simon **Gerber** (Paul Scherrer Institut):
X-Ray Free-Electron Lasers as a new Probe for Superconductors

15:00 Andrei **Pimenov** (TU Wien):
Modern Trends in Multiferroics

15:30 Coffee **Break**

16:00 Sandor **Bordacs**(Uni Budapest):
Toward the Understanding of Magnetoelectric Effect in BiFeO3

17:00 David **Szaller** (TU Wien):
Exotic Magnetoelectric Excitations of Multiferroic SmFe3(BO3)4

Evening session **Chair: Andrei Pimenov**

19:30 Evan **Constable** (TU Wien):
Magnetoelectric Effects in Fe Langasite

20:00 Lukas **Weymann** (TU Wien):
Magnetoelectric Properties and Tehahertz Dynamics in a Rare-Earth Langasite

Tuesday, 13.Feb. Chair: Peter Knoll

14:00 Franz **Giessibl** (Uni Regensburg):
Evidence of Bond Weakening Induced by Tip Proximity Studied by IETS and AFM

15:00 Short **Break**

15:15 Giovanni **Comelli** (Uni Trieste):
Graphene Growth on Ni Surfaces

16:15 **Coffee Break**

16:45 Yuri **Suchorski** (TU Wien):
Curved Microcrystals as Model Systems for Surface Reactions: H2Oxidation on Rh

Evening session **Chair: Peter Blaha**

19:30 Ulrike **Diebold** (TU Wien):
Atomic-Scale Investigations of Oxide Surfaces

20:00 Christian **Knoll** (TU Wien):
Investigations of the Reaction Kinetics of Thermochemical Energy Storage Materials

Friday, 16.Feb. Chair: Peter Weinberger

14:00 Olaf **Brummel** (FAU Erlangen-Nürnberg):
Electrocatalysis with Atomically-Defined Model Systems: Pt-Co3O4(111)

14:30 Magdalena **Bichler** (TU Wien):
The (012) Surfaces of Hematite – a DFT Study

15:00 Abdul **Motin** (TU Wien):
Hydrogenation on Carbon Supported Metal Clusters

15:30 **Coffee Break**

16:00 Annette **Foelske – Schmitz** (TU Wien):
X-Ray Photoelectron Spectroscopy of Ionic Liquids – From Half Cell Measurements to in Situ Electrochemical XPS Studies

16:30 Bonny **Dongre** (TU Wien)
Resonant Phonon Scattering in Semiconductors

17:00 Andreas **Tröster** (TU Wien)
Introduction to the Stress Tensor with DFT

Evening session **Chair: Günther Rupprechter**

19:30 Franz Renz (Leibniz Uni Hannover)
From Henry Walton Jones Jr. to Mark Watney

Wednesday, 14.Feb. Chair: Karlheinz Schwarz

14:00 Jan **Kotakoski** (Uni Vienna):
Structure and Manipulation of 2D Materials at the Atomic Level

15:00 Short **Break**

15:15 Florian **Libisch** (TU Wien):
Simulating Quantum Transport Trough Disordered Graphene Nanodevices

16:15 **Coffee Break**

16:45 Georg **Madsen** (TU Wien):
Transport in Defected Materials

Evening session **Chair: Peter Blaha**

19:30 **Poster session**:

Noelia Barrabes – Rabanal (TU Wien)
Insights on the Reactivity and Stability of Oxide Supported Aun(SR)m Clusters

Lorenz Bergen (TU Wien)
Phonon Spectroscopy of Magnetoelectric Langasite

Thomas Fabian (TU Wien)
An Efficient Basis set for Large – Scale Quantum Transport Calculations: Applications to Electron – Phonon Coupling

Georg Gravogel (TU Wien)
Moisture-triggered Carbonization of Main Group II Metal Oxides under Elevated CO_2 Pressure

Leila Kalantari (TU Wien)
Testing Nonlocal van der Waals Functionals for Layered Materials

Pawel Kulesza (University of Warsaw)
Development of Graphene-Based Supports for Platinum Catalysts Active at Low Loadings During Oxygen Reduction

Peter Kovacs (TU Wien)
Why Does SCAN Fail on Alkali Metals?

Alexander Liebig (University of Regensburg)
Coulomb´s Law at the Nanoscale: Imaging CaF_2(111) ba Atomic Force Microscopy With Atomically Characterized Tips

Franz Renz (University of Hannover)
Applied Molecular Switches in Drug Release and Gas Separation

Paolo Rudatis (TU Wien)
Reducing Graphene Oxide

Thomas Ruh (TU Wien)
The Delta-Project – Toward a Precision Benchmark Set for Solid State DFT

Günther Rupprechter (TU Wien)
SFG Spectroscopy at Atmospheric Pressure: CO oxidation on Pt/ZrO_2

Christopher Strablegg (University of Graz)
PECVD deposition and characterization of graphene layers

Dagmar Wengerowsky (Leibniz University Hannover)
The Hidden Klimt – An Analytical Approach