



## Program

### 35<sup>th</sup> Workshop

on

### *Novel Materials and Superconductors 2020*

**JUFA Schladming**

**February 09 – 14, 2020**

*Sponsored by TU Wien*

**Location**

JUFA Hotel Schladming  
Coburgstrasse 253, A – 8970 Schladming  
Tel: +43(0) 5/7083-330  
Fax: +43(0) 5/7083-331

**Date**

Arrival: Sunday, February 09th, 2020  
(Dinner 18:00, Get Together 19:30)  
Departure: Friday, February 14<sup>th</sup>, 2020

**Organizers:**

**Univ.Prof. Dr. Günther Rupprechter**

**Ao.Univ.Prof.Dr. Peter Blaha**

Institute of Materials Chemistry  
TU Wien, Getreidemarkt 9/E165, A-1060 Vienna  
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### Program Committee

B. Batlogg

P. Blaha

U. Diebold

F. Gießibl

P. Knoll

J.Kunze-Liebhäuser

S. Paschen

A. Pimenov

G. Rupprechter

K. Schwarz

P. Weinberger

<https://www.imc.tuwien.ac.at/konferenzen/>

## Scientific Program

### Monday, Feb. 10<sup>th</sup>, 2020 **Interface Science**

(Chair: **Ulrike Diebold**, TU Wien, Austria)

<b>14:00</b>	<b>Günther Rupprechter</b> (TU Wien, Austria) <i>Opening 35th Workshop</i>
<b>14:10</b>	<b>Introduction by Ulrike Diebold</b> (TU Wien, Austria)
<b>14:30</b>	<b>Peter Zeppenfeld</b> (JKU Linz, Austria) <i>Substrate-induced growth of organic thin films</i>
<b>15:10</b>	<i>Coffee Break</i>
<b>15:40</b>	<b>Martin Sterrer</b> (Univ. Graz, Austria) <i>Control of charge transfer through dielectric thin films</i>
<b>16:20</b>	<i>Coffee Break</i>
<b>16:40</b>	<b>Franz Gießibl</b> (Univ. Regensburg, Germany) <i>Cuddling atoms, subatomic resolution and physisorption-chemisorption transition seen by AFM</i>
<b>17:10</b>	<b>Break</b>

<b>18:00</b>	<b>Dinner</b>
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*Evening Session (Chair: Julia Kunze-Liebhäuser, Univ. Innsbruck, Austria)*

<b>19:30</b>	<b>Introduction by Julia Kunze-Liebhäuser</b> (Univ. Innsbruck, Austria)
<b>19:45</b>	<b>Jörg Libuda</b> (Univ. Erlangen, Germany) <i>Reducible Oxides: From model catalysis to model electrocatalysis</i>
<b>20:15</b>	<b>Nicola Seriani</b> (ICTP Trieste, Italy) <i>Ab-initio simulations of an electrochemical interface</i>
<b>20:45</b>	<b>End</b>

*For all talks: 5-10min discussion suggested !!*

**Tuesday, Feb. 11<sup>th</sup>, 2020 Spin crossover**

(Chair: Peter Weinberger, TU Wien, Austria)

<b>14:00</b>	<b>Introduction by Peter Weinberger</b> (TU Wien, Austria)
<b>14:20</b>	<b>Birgit Weber</b> (Univ. Bayreuth, Germany) <i>Synergy between spin state change and luminescence properties of 3d metal complexes</i>
<b>15:00</b>	<b>Coffee Break</b>
<b>15:30</b>	<b>Grace Morgan</b> (University College Dublin, Ireland) <i>Electronic and structural order parameter in spin switchable complexes</i>
<b>16:10</b>	<b>Refreshments</b>
<b>16:30</b>	<b>Marco Seifried</b> (TU Wien, Austria) <i>Substituted Azoles as potential ligands for iron SCO compounds</i>
<b>17:00</b>	<b>Break</b>
<b>17:00</b>	<b>Dinner</b>

*Evening Session (Chair: Peter Blaha, TU Wien, Austria)*

<b>19:30</b>	<b>Introduction by Peter Blaha</b> (TU Wien, Austria)
<b>19:45</b>	<b>Bernhard Bayer-Skoff</b> (TU Wien, Austria) <i>Resolving 2D/non-2D heterostructures</i>
<b>20:15</b>	<b>Meeting of the Program Committee</b>

**Wednesday, Feb. 12<sup>th</sup>, 2020 “Higgs”**

(Chair: Peter Knoll, Univ. Graz, Austria und Rudi Hackl, Walther-Meissner-Institut, Garching, Germany)

14:00	<b>Introduction by Peter Knoll</b> (Univ. Graz, Austria)
14:20	<b>Dirk van der Marel</b> (Univ. Geneve, Switzerland) <i>How to make photons massive with the help of a superconductor</i>
15:00	<b>Coffee Break</b>
15:30	<b>Ilse Krätschmer</b> (ÖAW HEPHY, Austria) <i>The God-damn particle</i>
16:10	<b>Refreshments</b>
16:30	<b>Marie-Aude Measson</b> (CNRS Neel Institute, France) <i>Higgs mode observability in charge-density-wave superconductors</i>
17:10	<b>Break</b>
18:00	<b>Dinner</b>

*Evening Session (Chair: Peter Blaha, TU Wien, Austria)*

**19:30 POSTER SHORT PRESENTATIONS AND POSTER SESSION**

**Thursday, Feb. 13<sup>th</sup>, 2020 Topological matter**

(Chair: Andrei Pimenov, TU Wien, Austria)

<b>14:00</b>	<b>Introduction by Andrei Pimenov</b> (TU Wien, Austria)
<b>14:20</b>	<b>Ronny Thomale</b> (Univ. Würzburg, Germany) <i>Room temperature quantum spin Hall effect</i>
<b>15:00</b>	<b>Coffee Break</b>
<b>15:30</b>	<b>Sergey Tarasenko</b> (Ioffe Institut, Russia) <i>Photogalvanic effects in 2D systems with non-trivial topology</i>
<b>16:10</b>	<b>Refreshments</b>
<b>16:30</b>	<b>Jan Gospodaric</b> (TU Wien, Austria) <i>A novel technique for obtaining band structures of 2D materials</i>
<b>17:00</b>	<b>Evan Constable</b> (TU Wien, Austria) <i>Magnetic monopoles in frustrated magnets</i>
<b>17:30</b>	<b>Break</b>

<b>18:00</b>	<b>Dinner</b>
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*Evening Session (Chair: Günther Rupprechter, TU Wien, Austria)*

<b>20:00</b>	<b>Bertram Batlogg</b> (ETH Zürich, Switzerland) <i>Physics in the Smartphone continued</i>
<b>21:00</b>	<b>Anna Pimenov</b> (TU Wien, Austria) <i>Kunst und Wissenschaft im Dialog</i> <i>techArt: Kunst im Labor</i>
<b>21:30</b>	<b>End</b>

**Friday, Feb. 14<sup>th</sup>, 2020 Nanomaterials**

(Chair: Günther Rupprechter, TU Wien, Austria)

14:00	<b>Introduction by Günther Rupprechter</b> (TU Wien, Austria)
14:20	<b>Erik Vesselli</b> (Università Trieste, Italy) <i>Tetrapyrroles in action at surfaces: an in situ approach</i>
15:00	<b>Coffee Break</b>
15:20	<b>Christophe Copéret</b> (ETH Zurich, Switzerland) <i>CO<sub>2</sub> hydrogenation to methanol: the role of surface and interfacial sites in controlling catalysis</i>
15:50	<b>Bert Chandler</b> (Trinity University, USA) <i>Small molecule activation at the Au-support interface</i>
16:20	<b>End</b>

***For all talks: 5-10min discussion suggested !!***

## **POSTER CONTRIBUTIONS**

### **Frustrated spin order and stripe fluctuations in FeSe**

A. Baum, H. N. Rziz, N. Lazarevic, Y. Wang, T. Böhm, R. H. Ahangharnejhad, P. Adelmann, T. Wolf, Z. V. Popovic, B. Moritz, T. P. Devereaux, R. Hackl

### **Far-Infrared dielectric response of antiferroelectric francisite Cu<sub>3</sub>Bi(SeO<sub>3</sub>)<sub>2</sub>O<sub>2</sub>Cl**

L. Bergen, L. Weymann, E. Malysheva, A. Pimenov, E. Constable

### **Are amorphous materials photocatalytically active? A case study with mesoporous niobium oxide**

L. Deilmann, T. Gupta, S. P. Nandan, D. Eder

### **Pressure dependence of low temperature carbonation of CaO under water saturation**

G Gravogl, F Birkelbach, D Müller, C. Lengauer, A. Werner, P. Weinberger, R. Miletich

### **Water adsorption on the CuOx and NiOx attached to the Anatase TiO<sub>2</sub>(101) surface by DFT Calculation**

L. Kalantari, P. Blaha

### **Combined STM/STS and AFM investigation on the topological insulator TiBiSe<sub>2</sub>**

A. Liebig, F. L. Kolb, F. J. Giessibl

### **Comparison of iron(II) and cobalt(II) complexes with imidazole-based scorpionate ligands**

F.M. Kapsamer, M. Seifried, G. Giester, J. Kunze-Liebhäuser, A. Auer, D. Müller, P. Weinberger

### **DFT Investigation of the effect of Ca doping on rare earth perovskites**

T. Ruh, L. Lindenthal, H. Summerer, R. Rameshan, A. K. Opitz, C. Rameshan, P. Blaha

### **In situ investigation of porphyrin reactivity at surfaces**

E. Vesselli, A. Verdini, S. Matus, F. Armillotta, J. Gallet, F. Bournelln

### **Field-induced linear magnetoelectric effect in a rare-earth langasite**

L. Weymann, T. Kain, A. Shuvaev, L. Bergen, E. Constable, Anna Pimenov, A. Kuzmenko, V. Yu. Ivanov, N. Kostyuchenko, D. Szaller, A. A. Mukhin, M. Mostovoy, A. Pimenov

### **Towards multifunctionality of a 4f-3d SCO complex**

W. Zeni, C. Knoll, M. Seifried, G. Giester, M. Reissner, D. Müller, P. Weinberger

### **Probing the electronic structure using resonant light scattering**

R. Hackl, A. Baum, N. Lazarevic, Y. Li, C.-H. Chu, I.R. Fisher, R. Valenti, I.I. Mazin

**Gold nanoclusters for oxidation reactions: Size, support and doping effects on catalytic activity**

C. Garcia, N. Barabas, G. Rupprechter

**Active site structures in Titanium-Silicalite 1: An NMR point of view**

C. P. Gordon, H. Engler, A. Berkessel, J.H. Teles, A. N. Parvulescu, C. Copéret

**Catalytic Interfaces for photoelectrochemical and electrochemical reduction of Carbon Dioxide**

P. J. Kulesza, I. A. Rutkowska,

**Catalytic Processes of highly inert systems in acid medium: Detection of As(III) and As(V)**

A. Rutkowska, P. J. Kulesza,

**Terahertz time-domain spectroscopy at low temperatures**

J. Wettstein, D. Szaller, E. Constable, A. Pimenov

**Chiral Fe(II) spin crossover complexes based on the BINOL motif**

M. Nastran, D. Müller, W. Zeni, M. Seifried, P. Weinberger

**Quantum-optical phenomena in magnetoelectric crystals**

D. Szaller, J. Wettstein, K. Amelin, T. Room, U. Nagel, A. Kuzmenko, A. Pimenov

**Iron and the “Putto”**

D. Wengerowsky, R. Lehmann, H.-J. Schmidt, M. Kumar, R. Sindelar, B.F.O. Costa, F. Renz

**Mixed valance multinuclear complexe: Spin Transition**

D. Natke, J. Pawlak, A. Preiss, H. Oshio, R. Sindelar, F. Renz

**Constructing the phase diagram of HfO<sub>2</sub> using artificial intelligence and first principles calculations**

S. Bichelmaier, J. Carrete, G.K.H. Madsen

***General Information:***

*Breakfast: 07.00 – 10.30*

*Lunch: 12.30 – 13:15*

*Dinner: 18.00 – 20.00*

## Anreise

Mit Bus oder Bahn:

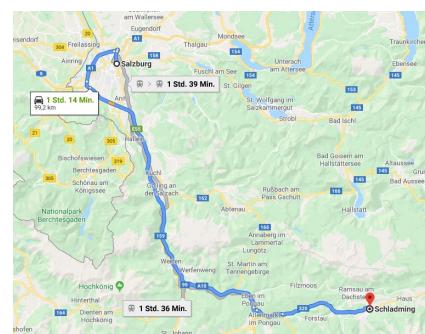
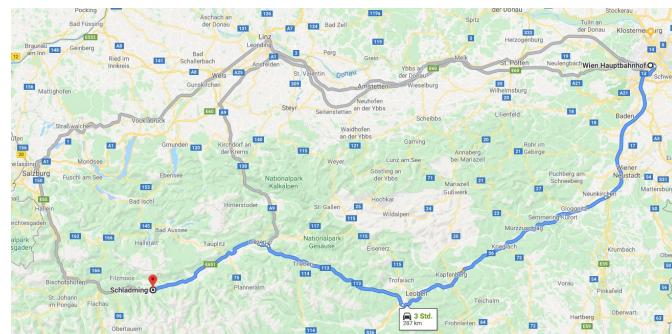
Von Salzburg Stadt – Schladming 1h36min

Von Wien HBF – Schladming 4h30min

Fußweg vom Bahnhof zum Jufa Hotel ca. 15 min



Mit dem Auto :



### Aus Wien:

A23 Richtung bis

Süd Autobahn/E59, S6 und A9 bis B320 in  
Selzthal folgen

A9 Ausfahrt B320 nehmen 2 Std. 9 Min. (230 km)  
B320 bis Roseggerstraße in Schladming

### Aus Salzburg:

A1 nehmen bis

A10 bis Anschlußstelle

Ennstal/B320/E651 nehmen

A10 Ausfahrt 63-Altenmarkt nehmen

B320 bis Roseggerstraße in  
Schladming folgen