



TECHNISCHE
UNIVERSITÄT
WIEN



Program



33. Workshop

on

Novel Materials and Superconductivity

BSFZ Obertraun

11. - 17. February 2018

Sponsored by TU Wien

Location:	Bundessportheim und Freizeitzentrum BSFZ Obertraun Winkl 49 (Oberösterreich, A – 4831 Obertraun Tel: [+43] (6131) 239-0 international Fax: [+43] (6131) 239-423 international
Date:	Arrival: Sunday, February 11th, 2018 (Dinner 18:00, Get Together 19:30) Departure: Saturday, February 17th, 2018

Organizers:

Univ.Prof. Dr. Günther Rupprechter

Ao.Univ.Prof.Dr. Peter Blaha

Mag.phil. Ulrike Prohaska

Institute of Materials Chemistry

TU Wien, Getreidemarkt 9/E165, A-1060 Vienna

Tel: [+43] (1) 58801-165101

Fax: [+43] (1) 58801-16599

E-Mail: guenther.rupprechter@tuwien.ac.at

Programme Committee:

B. Batlogg

U. Diebold

P. Knoll

F. Kubel

W. Lang

S. Paschen

G. Rupprechter

K. Schwarz

P. Weinberger

World Wide Web: <http://wien2k.at/theochem/obertraun/>

Scientific Program

Monday, Feb. 12th, 2018 *Thermal-, Photo- and Electro-Catalysis*

(Chair: Günther Rupprechter)

- 14:00** **Günther Rupprechter** (TU Wien, Austria)
Opening 33rd Workshop
- 14:10** **Thomas Bürgi** (University of Geneva, Switzerland)
On the Reactivity of Monolayer-Protected Metal Clusters
- 15:10** **Short Break**
- 15:30** **Gerhard Mestl** (Clariant, Germany)
High-Throughput Optimization of Catalytic Materials
- 16:30** **Coffee Break**
- 17:00** **Alexey Cherevan** (TU Wien, Austria)
State-of-the-art, Challenges and Prospects of Photocatalysis
- 18:00** **Break**

18:15 **Dinner**

Evening Session (Chair: Ulrike Diebold)

- 19:30** **Julia Kunze – Liebhäuser** (University of Innsbruck, Austria)
N. Shakibi-Nia, D. Hochfilzer, E.M. Wernig, J. Kunze-Liebhäuser
Electro-Activation of Small Molecules at the Solid/Liquid Interface
- 20:00** **Iwona Rutkowska** (University of Warsaw, Poland)
I.A. Rutkowska, P.J. Kulesza
Mixed – Metal Oxide Supports for Efficient Electrocatalysis
- 20:30** **End**

Tuesday, Feb. 13th, 2018 *Surface Science*

(Chair: Peter Knoll)

14:00 Franz Giessibl (University of Regensburg, Germany)

N. Okabayashi, A. Peronio, M. Paulsson, T. Arai, F. J. Giessibl

Evidence of Bond Weakening Induced by Tip Proximity Studied by IETS and AFM

15:00 Short Break

15:15 Giovanni Comelli (University of Trieste, Italy)

Graphene Growth on Ni Surfaces

16:15 Coffee Break

16:45 Yuri Suchorski (TU Wien, Austria)

Curved Microcrystals as Model Systems for Surface Reactions: H₂ Oxidation on Rh

17:45 Break

18:15 Dinner

Evening Session (Chair: Peter Blaha)

19:30 Ulrike Diebold (TU Wien, Austria)

Atomic-Scale Investigations of Oxide Surfaces

20:00 Christian Knoll (TU Wien, Austria)

C. Knoll, D. Müller, G. Gravogl, W. Artner, A. Werner, M. Harasek, P. Weinberger, T. Ruh, P. Blaha

Investigations of the Reaction Kinetics of Thermochemical Energy Storage Materials

20:30 End

Wednesday, Feb. 14th, 2018 *Novel Materials and Simulations*

(Chair: Karlheinz Schwarz)

14:00 **Jan Kotakoski** (University of Vienna, Austria)

Structure and Manipulation of 2D Materials at the Atomic Level

15:00 **Short Break**

15:15 **Florian Libisch** (TU Wien, Austria)

Simulating Quantum Transport Through Disordered Graphene Nanodevices

16:15 **Coffee Break**

16:45 **Georg Madsen** (TU Wien, Austria)

Transport in Defected Materials

17:45 **Break**

18:15 **Dinner**

Evening Session (Chair: Peter Blaha)

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

Thursday, Feb. 15th, 2018 *Superconductors and Multiferroics*

(Chair: Bertram Batlogg)

14:00 **Simon Gerber** (Paul Scherrer Institut, Switzerland)

X-Ray Free-Electron Lasers as a new Probe for Superconductors

15:00 **Andrei Pimenov** (TU Wien, Austria)

Modern Trends in Multiferroics

15:30 **Coffee Break**

16:00 **Sandor Bordacs** (Budapest University of Technology and Economics, Hungary)

S. Bordacs, D. Farkas, D. Szaller, U. Nagel, T. Room, T. Ito, I. Kezsmarki

Toward the Understanding of Magnetoelectric Effect in BiFeO_3

17:00 **David Szaller** (TU Wien, Austria)

D. Szaller, A.M. Kuzmenko, Th. Kain, L. Weymann, A. Shuvaev, Anna Pimenov, A.A. Mukhin, V. Yu. Ivanov, I.A. Gudim, L.N. Bezmaternykh, A. Pimenov

Exotic Magnetoelectric Excitations of Multiferroic $\text{SmFe}_3(\text{BO}_3)_4$

17:30 **Break**

18:15 **Dinner**

Evening Session (Chair: Andrei Pimenov)

19:30 **Evan Constable** (TU Wien, Austria)

E. Constable, V. Simonet, C.V. Colin, S. de Brion, E. Ressouche, F. Gay, R. Ballou, P. Lejay, A. Cano

Magnetoelectric Effects in Fe Langasite

20:00 **Lukas Weymann** (TU Wien, Austria)

L. Weymann, Th. Kain, A. Shuvaev, A.A. Mukhin, I.A. Gudim, L.N. Bezmaternykh, A. Pimenov

Magnetoelectric Properties and Terahertz Dynamics in a Rare-Earth Langasite

20:30 **End**

Friday, Feb. 16th, 2018 *Impulse Presentations*

(Chair: Peter Weinberger)

- 14:00** **Olaf Brummel** (FAU Erlangen-Nürnberg, Germany)
O. Brummel, F. Faisal, C. Stumm, M. Bertram, Y. Lykhach, J. Libuda
*Electrocatalysis with Atomically-Defined Model Systems:
Pt-Co₃O₄(111)*
- 14:30** **Magdalena Bichler** (TU Wien, Austria)
M. Bichler, P. Blaha
The (012) Surfaces of Hematite – a DFT Study
- 15:00** **Abdul Motin** (TU Wien, Austria)
A.Md. Motin, C. Rameshan, G. Rupprechter
Hydrogenation on Carbon Supported Metal Clusters
- 15:30** **Coffee Break**
- 16:00** **Annette Foelske – Schmitz** (TU Wien, Austria)
*X-Ray Photoelectron Spectroscopy of Ionic Liquids - From Half Cell
Measurements to in Situ Electrochemical XPS Studies*
- 16:30** **Bonny Dongre** (TU Wien, Austria)
B. Dongre, J. Carrete, A. Katre, N. Mingo, G. Madse
Resonant Phonon Scattering in Semiconductors
- 17:00** **Andreas Tröster** (TU Wien, Austria)
Introduction to the Stress Tensor with DFT
- 17:30** **End**

18:15 **Dinner**

Evening Session (Chair: Günther Rupprechter)

- 19:30** **Franz Renz** (Leibniz Universität Hannover, Germany)
From Henry Walton Jones Jr. to Mark Watney

POSTER CONTRIBUTIONS:

- **Noelia Barrabes – Rabanal** (TU Wien)
N. Barrabés, S. Pollitt, G. Rupprechter
Insights on the Reactivity and Stability of Oxide Supported $Au_n(SR)_m$ Clusters
- **Lorenz Bergen** (TU Wien)
L. Bergen, E. Constable, L. Weymann, A.A. Mukhin, I.A. Gudim, L.N. Bezmaternykh, Anna Pimenov, A. Pimenov
Phonon Spectroscopy of Magnetoelectric Langasite
- **Thomas Fabian** (TU Wien)
T. Fabian, J. Burgdörfer, F. Libisch
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)
L. Kalantari, F. Tran, P. Blaha
Testing Nonlocal van der Waals Functionals for Layered Materials
- **Pawel Kulesza** (University of Warsaw)
P.J. Kulesza, I.A. Rutkowska, S. Zoladek, B. Dembinska, K. Miecznikowski
Development of Graphene-Based Supports for Platinum Catalysts Active at Low Loadings During Oxygen Reduction
- **Peter Kovacs** (TU Wien)
P. Kovacs
Why Does SCAN Fail on Alkali Metals?
- **Alexander Liebig** (University of Regensburg)
A.Liebig, A. Peronio, D. Meuer, A.J. Weymouth, F. J. Giessibl
Coulomb’s Law at the Nanoscale: Imaging $CaF_2(111)$ by Atomic Force Microscopy With Atomically Characterized Tips
- **Franz Renz** (University of Hannover)
M. Kumar, D. Wengerowsky, D. Unruh, R. Sindelar, G. Klingelhöfer, F. Renz
Applied Molecular Switches in Drug Release and Gas Separation

- **Paolo Rudatis** (TU Wien)
P. Rudatis, J. Binting, A. Cherevan, H. Mikula, D. Eder
Reducing Graphene Oxide
- **Thomas Ruh** (TU Wien)
T. Ruh, K. Lejaeghere, S. Cottenier, P. Blaha
The Delta-Project – Toward a Precision Benchmark Set for Solid State DFT
- **Günther Rupprechter** (TU Wien)
V. Pramhaas, M. Roiaz, X. Li, C. Rameshan, G. Rupprechter
SFG Spectroscopy at Atmospheric Pressure: CO oxidation on Pt/ZrO₂
- **Christopher Strablegg** (University of Graz)
C. Strablegg, J. Reyvvaan, M. Mayer, P. Knoll
PECVD deposition and characterization of graphene layers
- **Dagmar Wengerowsky** (Leibniz University Hannover)
D. Wengerowsky, M. Kumar, F. Renz
The Hidden Klimt – An Analytical Approach

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 Terahertz 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 Au(SR)_n 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 CO₂ 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 CaF₂(111) by 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/ZrO₂

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

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

List of participants

33 . Workshop

07.02.2018

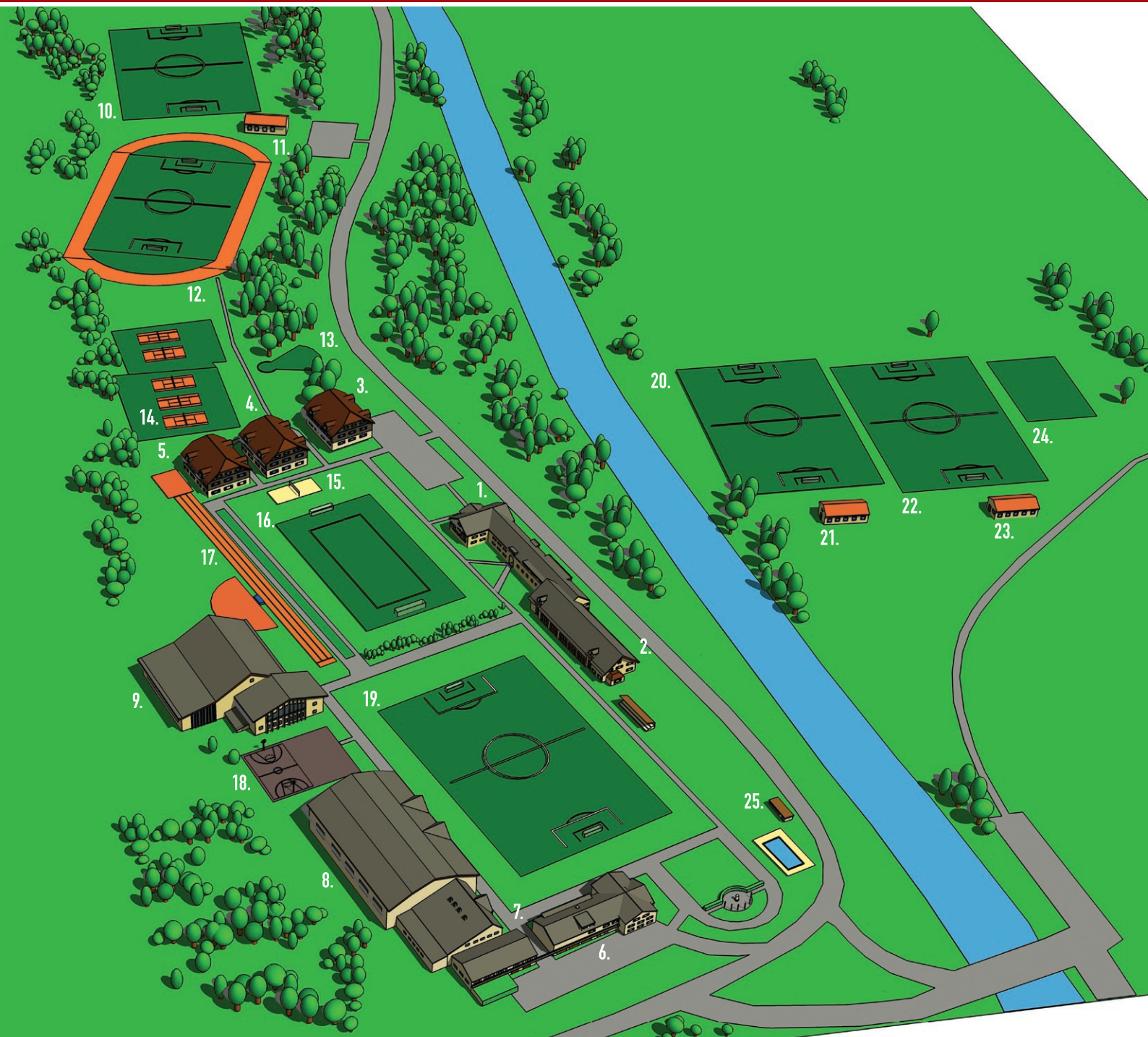
first name	last name	Institution	BSFZ	Room Number
Bertram	Batlogg	ETH Zürich, CH	1	527
Hadi	Batlogg		1	527
Lorenz	Bergen	TU Wien - E138, AUT	1	511
Magdalena	Bichler	TU Wien - E165, AUT	1	412
Peter	Blaha	TU Wien - E165, AUT	1	506
Evelin	Boller		1	526
Herbert	Boller	JKU Linz, AUT	1	526
Sandor	Bordacs	Univ. Budapest, HU	1	512
Olaf	Brummel	FAU Erlangen, GER	1	502
Thomas	Bürgi	Univ. Geneva, CH	1	408
Alexey	Cherevan	TU Wien - E165, AUT	1	509
Giovanni	Comelli	Univ. Trieste, IT	1	523
Evan	Constable	TU Wien - E138, AUT	1	413
Ulrike	Diebold	TU Wien - E134, AUT	1	411
Bonny	Dongre	TU Wien - E165, AUT	1	522
Jan	Doumont	TU Wien - E165, AUT	1	522
Thomas	Fabian	TU Wien - E136, AUT	1	418
Annette	Foelske-Schmitz	TU Wien - AIC, AUT	1	514
Simon	Gerber	PSI, Villigen, CH	1	502
Franz	Giessibl	Univ. Regensburg, GER	1	414
Valentin	Giessibl		1	501
Birgit	Giessibl		1	414
Georg	Gravogl	TU Wien - E163, AUT	1	417
Leila	Kalantari	TU Wien - E165, AUT	1	513
Christian	Knoll	TU Wien - E163, AUT	1	417
Peter	Knoll	Univ. Graz, AUT	1	506
Jani	Kotakoski	Univ. Vienna, AUT	1	524
Peter	Kovacs	TU Wien - E165, AUT	1	413
Frank	Kubel	TU WIEN - 164, AUT	1	416
Pawel	Kulesza	Univ. Warsaw, PL	1	415
Julia	Kunze-Liebäuser	Univ. Innsbruck, AUT	1	514
Florian	Libisch	TU Wien - E136, AUT	1	508
Alexander	Liebig	Univ. Regensburg, GER	1	501
Georg	Madsen	TU Wien - E165, AUT	1	503
Gerhard	Mestl	Clariant, GER	0	
Abdul Md.	Motin	TU Wien - E165, AUT	1	524
Anna	Pimenov	TU Wien - E138, AUT	1	507
Andrei	Pimenov	TU Wien - E138, AUT	1	507
Gerhard	Piringer	Univ. Bodenkultur, AUT	1	411
Franz	Renz	Leibniz Univ. Hannover, GER	1	510
Sonja	Reitschmidt		1	412
Paolo	Rudatis	TU Wien - E165, AUT	1	509
Thomas	Ruh	TU Wien - E165, AUT	1	417
Günther	Rupprechter	TU Wien - E165, AUT	1	504
Iwona	Rutkowska	Univ. Warsaw, PL	1	415
Christine	Schwarz		1	525
Karlheinz	Schwarz	TU Wien - E165, AUT	1	525
Jenny	Stein	Univ. Bodenkultur, AUT	1	410
Thomas	Stein	Univ. Bodenkultur, AUT	1	410
Conrad	Stein	Univ. Bodenkultur, AUT	1	410
Christopher	Strablegg	Univ. Graz, AUT	1	418
Yuri	Suchorski	TU Wien - E165, AUT	1	505
David	Szaller	TU Wien - E138, AUT	1	512
Andreas	Tröster	TU Wien - E165, AUT	1	508
Dagmar	Wengerowsky	Leibniz Univ. Hannover, GER	1	513
Peter	Weinberger	TU Wien - E163, AUT	1	521
Lukas	Weymann	TU Wien - E138, AUT	1	511
				56

Grant

external Guest

ROOMNUMBERS 408 - 418 House "Saarstein"

ROOMNUMBERS 501 - 527 House "Dachstein"



1. Haus Sarstein, Rezeption, Zimmer • 2. Restaurant, Sportcafe • 3. Haus Aussee • 4. Haus Obertraun • 5. Haus Hallstatt
 • 6. Haus Dachstein • 7. Sportgeräteausgabe, Schiverleih • 8. Dreifach-Halle, Kraftkammer, Gymnastikraum, Tischtennis
 • 9. Halle 1, Halle 2, Sauna, Kletterraum, Seminarraum • 10. Kunstrasenplatz 1 • 11. Garderobengebäude • 12. Fußballplatz 2,
 LA-Anlage, 400-Meter Bahn • 13. Kugelstoßanlage • 14. Tennisplätze • 15. Beachvolleyball-platz • 16. Kunstrasenplatz 2
 • 17. 60-Meter Bahn, Sprunggrube, Hochsprunganlage • 18. Asphalt-Ballsplatz • 19. Fußballplatz 1 • 20. Fußballplatz 4
 • 21. Garderobengebäude • 22. Fußballplatz 3 • 23. Garderobengebäude • 24. Faustballplatz • 25. Beheiztes Freischwimm-
 becken