RUPPRECHTER, Günther

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Education

- 2005: Habilitation for Physical Chemistry, Technical University Berlin, Germany.
- 1996: Ph.D. Chemistry (Dr. rer. nat.), summa cum laude, University Innsbruck, Austria.
- 1992: M.Sc. Chemistry (Mag. rer. nat.), summa cum laude, University Innsbruck, Austria.

Work experience

- 2010-present: Head of the Institute of Materials Chemistry, TU Wien.
- 2005-present: Full Professor (Chair) of Surface & Interface Chemistry, IMC, TU Wien, Austria.
- 1998-2006: Group Leader for Laser Spectroscopy & Catalysis at the Fritz Haber Institute, Max Planck Society, Chemical Physics Department, Berlin, Germany (with H.-J. Freund).
- 1996-1998: Postdoctoral Fellow at the Department of Chemistry, University of California at Berkeley and E.O. Lawrence Berkeley National Laboratory (with G.A. Somorjai).

Experience in leading large cooperative research projects

From 2011 to 2019, Günther Rupprechter was Speaker/Coordinator of the FWF-funded Special Research Program (SFB) "Functional Oxide Surfaces and Interfaces (FOXSI)", involving 150 researchers in 10 research groups (total budget of ~8.4 Mio €). He also directed the TU Wien Doctorate school "Catalysis Materials and Technology" with 11 research groups from 2011 to 2014. Günther Rupprechter is "Director of Research" (Speaker) of the FWF-funded Cluster of Excellence "Materials for Energy Conversion and Storage (MECS)", including 19 research groups at 4 universities. The COE MECS (34.43 Mio €, 2023-2028, with an option of extension to 2033) is one of three COEs in the natural sciences (among five first Clusters of Excellence in Austria).

Research interests

Research is focused on catalytic surface reactions on heterogeneous catalysts, employing a three-pronged approach: (i) surface-science-based planar model catalysts, (ii) atomically-precise clusters, and (iii) industrial-grade nanomaterials. Elucidating, among others, molecular mechanisms of hydrogen as clean fuel, methane reforming, CO_2 and olefin hydrogenation, efficient automotive catalysis, and waste remediation. Materials include mono- (Pt, Pd, Rh, Cu, Ni, Au, Co) and bimetallic (PdZn, Pd_2Ga, PdCu, CuNi, CuZn, PdAu, AgAu, CuAu, RhAu) nanoparticles on supporting (mixed) oxides (Al_2O_3, SiO_2, CeO_2, PrO_2, ZrO_2, TiO_2, ZnO, MgO, Ga_2O_3, Co_3O_4), perovskites (LCO, LSF), and carbon (HOPG, GR).

As examining functioning catalysts at near atmospheric pressure (NAP) and realistic temperature is crucial, dedicated UHV-compatible high-pressure cells have been developed for model catalysts (single crystals, thin films, nanoparticles), enabling sum frequency generation (SFG) laser spectroscopy, polarization-modulation infrared reflection absorption spectroscopy (PM-IRAS), and X-ray photoelectron spectroscopy (NAP-XPS) under reaction conditions. Corresponding *in situ* (*operando*) spectroscopy of nanomaterials is carried out by Fourier transform infrared spectroscopy (FTIR), X-ray absorption spectroscopy (XAS), NAP-XPS, and X-ray diffraction (XRD). Significant advances were made in imaging the local kinetics of surface reactions by *in situ surface (correlative) microscopy*, with photoemission electron microscopy (PEEM), scanning photo-electron microscopy (SPEM) and field emission/ion microscopy (FEM/FIM) applied to metals and metal/oxide interfaces. Most studies were carried out at synchrotron sources and in lock-step with theory collaborations (DFT and microkinetics).

Most relevant scientific results (*[numbers] refer to the key publications below*):

- Fundamentals and applications of (near) ambient pressure surface spectroscopy (SFG/PM-IRAS/NAP-XPS/XAS/DRIFTS) were summarized in several review articles that exemplified the power of *in situ* and *operando* studies of catalytic reactions (e.g. [1, 2]).
- **Model Catalysis:** I am among the early researchers in ambient pressure surface science, developing and applying UHV-compatible high-pressure (HP) cells for combined *in situ surface spectroscopy* and kinetics [1, 2]: SFG with G.A. Somorjai, SFG/PM-IRAS with H.-J. Freund, NAP-XPS with V.I. Bukhtiyarov. This enabled atmospheric pressure studies of UHV-grown model systems, creating the vital link to technolgical catalysis. Among several constructed HP cells, one specific design is used by several groups worldwide.
- **Model Catalysis:** Very first paper of SFG spectroscopy on oxide supported Pd nanoparticles, demonstrating size and pressure (UHV to mbar) effects in CO adsorption [3]. This triggered many follow-up studies, also combined with NAP-XPS (JPC B 2003/2004, Appl. Surf. Sci. 2004). My SFG activities continue till today, including single crystals (Top. Catal. 2018), thin films, and nanoparticles [4, 5].
- **Model Catalysis:** Combining atmospheric pressure reaction kinetics of the complex 1-butene hydrogenation and isomerization on Pd single crystals and Pd/Al_2O_3 model catalysts with DFT calculations and microkinetic modeling (with A. Genest and N. Rösch), the particle size-dependent selectivity could be rationalized based on the abundance and specific properties of the contributing nanoparticle facets [6,7].
- **Model & Applied Catalysis:** Molecular-level *operando* insights into selective methanol steam reforming on PdZn and PdGa intermetallics (NAP-XPS, PM-IRAS, concentration modulation IR, EXAFS, DFT; with B. Klötzer, D. Ferri, K.M. Neyman) [2]. We were able to link reaction selectivity to the catalyst´s atomic and electronic (VB) structure, backed by DFT (JPC C 2015). Model and applied studies blended well together.
- **Model and Applied Catalysis**: Studies of ZrO_2-based reforming catalysts by *in situ* (synchrotron) NAP-XPS and XAS spectroscopy, employing ultrathin (trilayer) ZrO_2 films (Surf. Sci. 2019, JPC C 2015) and nanopowders of ZrO_2 and ZrO_2/CeO_2 (Catal. Tod. 2016/2017). Further studies of methane dry reforming demonstrated SMSI effects (J. Phys. Cond. Matt. 2018), Ni surface segregation in bimetallic $CuNi/ZrO_2$, and coke suppression for $Ni/ZrO_2/CeO_2$ [2].
- **Applied Catalysis**: Operando surface spectroscopy (XAS, NAP-XPS, FTIR, XRD) of CO oxidation and PROX on Co_3O_4 catalysts, exploiting both static and dynamic conditions, revealed a complex reaction network [2, 8]. The presumably active (oxygen vacancy) sites were a minority species. Further studies contrasted Co_3O_4 to Co_3O_4/CeO_2 and CoO (J. Phys.: Cond. Matt. 2022, Chem. Europ. J. 2021, Catal. Tod. 2019).
- **Applied Catalysis**: Surface chemistry of Au clusters on ceria-praseodymia mixed oxide supports: $Au/Ce_4Pr_1O_x$ exhibited the highest activity in water gas shift, with combined experimental and theoretical studies showing that asymmetric O vacancies facilitate H_2O dissociation [9]. Using thiloate-protected atomically-precise Au clusters on various supports as truly monodisperse catalysts [10].
- **In situ/operando Surface Microscopy:** Locally-resolved imaging of ongoing surface reactions by PEEM, directly revealing phenomena such as facet-resolved catalytic ignition, multi-frequential oscillations, anisotropic surface oxidation, coexisting multi-states, and long-ranging metal/oxide interface effects (with Y. Suchorski) [2, 11, 12]. This opened a new pathway to investigate catalyst heterogeneity and structure sensitivity, based on a 10-year research effort in developing the concepts of *kinetics by imaging* and *surface structure and particle size libraries*. Combining PEEM and DFT/microkinetics (with K.M. Neyman and H. Grönbeck) yielded fundamental insights on interface activity [11]. PEEM was combined with SPEM (Scanning Photoelectron Microscopy) [12] and recently extended to XPEEM and LEEM (low energy electron microscopy) in a true *in situ correlative microscopy* approach (ACS Catalysis 2022).
- **Single Particle Catalysis**: Field electron microscopy (FEM) is applied to image an ongoing catalytic reaction on an individual metal nanocrystal in real time, enabling to resolve interfacet coupling and its collapse due to restructuring [13]. When the ionized water product was used as imaging species, the active sites were directly identified by *in situ* field ion microscopy (FIM). First observation of nano-chaos in a catalytic reaction [14] and direct imaging of rare-earth promotor effects [15].

Selected key publications (for full list, incl. 13 book chapters, see ORCID, Web of Science or Google Scholar)

1. G. Rupprechter
Sum frequency generation and polarization-modulation infrared reflection absorption spectroscopy of functioning model catalysts from ultrahigh vacuum to ambient pressure
Advances in Catalysis, 51 (2007) 133-263

2. G. Rupprechter
Operando surface spectroscopy and microscopy during catalytic reactions: from clusters via nanoparticles to meso-scale aggregates
Small, 2004289 (2021) 26p

3. T. Dellwig, G. Rupprechter, H. Unterhalt, H.-J. Freund
Bridging the pressure and materials gaps: High pressure sum frequency generation study on supported Pd nanoparticles
Physical Review Letters 85 (2000) 776-779

4. V. Pramhaas, M. Roiaz, N. Bosio, C. Rameshan, M. Corva, E. Vesselli, H. Grönbeck, G. Rupprechter
Interplay between CO disproportionation and oxidation: on the origin of the CO reaction onset on Atomic Layer Deposition-grown Pt/ZrO_2 model catalysts
ACS Catalysis, 11 (2021) 208–21

5. V. Pramhaas, H. Unterhalt, H.-J. Freund, G. Rupprechter
Polarization-dependent sum frequency generation (SFG) spectroscopy for in situ tracking of nanoparticle morphology
Angewandte Chemie International Edition, e202300230 (2023)

6. V. Markova, J. Philbin, W. Zhao, A. Genest, J. Silvestre-Albero, G. Rupprechter, N. Rösch
Catalytic transformations of 1-Butene over palladium. A combined experimental and theoretical study
ACS Catalysis 8 (2018) 5675-5685

7. A. Genest, J. Silvestre-Albero, W.-Q. Li, N. Rösch, G. Rupprechter
The origin of the particle-size-dependent selectivity in 1-butene isomerization and hydrogenation on Pd/Al_2O_3 catalysts
Nature Communications, 12 (2021) 6098 (8 pages)

8. L. Lukashuk, N. Yigit, R. Rameshan, E. Kolar, D. Teschner, M. Hävecker, A. Knop-Gericke, R. Schlögl, K. Föttinger, G. Rupprechter
Operando insights into CO oxidation on cobalt oxide catalysts by NAP-XPS, FTIR and XRD
ACS Catalysis 8 (2018) 8630−8641

9. J. Shi, H. Li, A. Genest, W. Zhao, P. Qi, T. Wang, G. Rupprechter
High-performance water gas shift induced by asymmetric oxygen vacancies: Gold clusters supported by ceria-praseodymia mixed oxides
Applied Catalysis B: Environmental, 301 (2022) 120789

10. S. Pollitt, V. Truttmann, T. Haunold, C. Garcia, W. Olszewski, J. Llorca, N. Barrabés, G. Rupprechter
The dynamic structure of $Au_{38}(SR)_{24}$ nanoclusters supported on CeO_2 upon pretreatment and CO oxidation
ACS Catalysis, 10 (2020) 6144−6148

11. Y. Suchorski, S.M. Kozlov, I. Bespalov, M. Datler, D. Vogel, Z. Budinska, K.M. Neyman, G. Rupprechter
The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation
Nature Materials, 17 (2018) 519-522

12. P. Winkler, J. Zeininger, Y. Suchorski, M. Stöger-Pollach, P. Zeller, M. Amati, L. Gregoratti, G. Rupprechter
How the anisotropy of surface oxide formation influences the transient activity of a surface reaction
Nature Communications, 12 (2021) 69

13. Y. Suchorski, J. Zeininger, S. Buhr, M. Raab, M. Stöger-Pollach, J. Bernardi, H. Grönbeck, G. Rupprechter
Resolving multifrequential oscillations and nanoscale interfacet communication in single particle catalysis
Science, 372 (2021) 1314-1318

14. M. Raab, J. Zeininger, Y. Suchorski, K. Tokuda, G. Rupprechter
Emergence of chaos in a compartmentalized catalytic reaction nanosystem
Nature Communications, 14 (2023) 282

15. M. Raab, J. Zeininger, Y. Suchorski, A. Genest, C. Weigl, G. Rupprechter
Lanthanum modulated reaction pacemakers on a single catalytic nanoparticle
Nature Communications, 14 (2023) 7186

Most recent, other achievements

1. Guest Professor at Kasetsart University Bangkok, Thailand (2023). Distinguished Overseas Professorship of Shanghai University of Engineering Science (SUES), China (2018-2022).
2. Jochen Block Award of the German Catalysis Society (DECHEMA) "for the application of surface science methods to heterogeneous catalysis" (2005).
3. Corresponding Member of Austrian Academy of Sciences (2012). Fellow of the European Academy of Sciences (2023).
4. Member of Panel PE4 (Physical and Analytical Chemical Sciences) for Consolidator Research Grants of the European Research Council, ERC (2014&2016&20182020) and Member of the ESRF (European Synchrotron Radiation Facility) Board of ÖAW (2014-2023). Various Award Panels of ÖAW (2017–2023).
5. Speaker of the FWF Special Research Program (SFB) "Functional Oxide Surfaces and Interfaces (FOXSI)" (2011-2019), PI of FWF SFB "Taming Complexity in Materials Modeling (TACO)" (2021–). "Director of Research" (Speaker) of the FWF-funded Cluster of Excellence "Materials for Energy Conversion and Storage (COE MECS) (2023-)".
6. Editorial Board Member of *Catalysis Letters* and *Topics in Catalysis* (2011–).
7. Leadership roles in professional Societies such as *Austrian Chemical Society* (GÖCH), *Section Surface Chemistry and Catalysis* (Chair 2006 – 2016, Vice Chair 2016 – 2023) and *Chemical Physical Society* (Board/Chair 2009-2012).
8. Organizer (Chair) of the annual "International Workshop on Novel Materials and Superconductivity" (with P. Blaha), Schladming, Austria (50-70 participants, 2018 – 2024). Organizer of an EFCATS Summer School "Engineering Materials for Catalysis" (with Albin Pintar and Nataša Novak Tušar), Portorož-Portorose, Slovenia (about 60 participants; September 2020). Scientific Committee of the Faraday Discussion on "Photoelectron Spectroscopy: New Horizons in Surface Analysis", London, UK (with about 100 participants, April 2022).
9. About 265 peer reviewed publications (10 Nature Journals, 1 Science, 4 ACiE, 9 ACS Catalysis, 6 Appl. Catal. B, 1 PRL), Number of citations: ~8,700 (Web of Science), ~12,000 (Google Scholar).
10. Invited talks: 162 at conferences/colloquia, incl. 30 plenary/keynote lectures, with 5 named lectures.
11. Supervised 25 Post-docs and 29 Ph.D. students, 8 now hold academic positions at various ranks.