Publications

Ordered by Project Parts

Joint Publications within the SFB are marked by the involved project parts (after the title, simply in numerical order, e.g. **P01/02/04**).

Project Part 01 Coordination Project (including USTEM and DESY)

An ultra-flexible modular high vacuum setup for thin film deposition
T. Götsch, E.-M. Wernig, B. Klötzer, T. Schachinger, J. Kunze-Liebhäuser, S. Penner
Review of Scientific Instruments 90 (2019) 023902-1 – 023902-13
https://doi.org/10.1063/1.5065786 (Green OA)

Crystallographic and electronic evolution of lanthanum strontium ferrite ($La_{0.6}Sr_{0.4}FeO_{3-\delta}$) thin film and bulk model systems during iron exsolution **P01/03**
T. Götsch, N. Köpfle, M. Grünbacher, J. Bernardi, E. A. Carbonio, M. Hävecker, A. Knop-Gericke, M. F. Bekheet, L. Schlicker, A. Doran, A. Gurlo, A. Franz, B. Klötzer, S. Penner
Physical Chemistry Chemical Physics 21 (2019) 3781-3794
https://doi.org/10.1039/c8cp07743f (Green OA)

On the structural stability of crystalline ceria phases in undoped and acceptor-doped ceria materials under in situ reduction conditions
M. F. Bekheet, M. Grünbacher, L. Schlicker, A. Gili, A. Doran, J. D. Epping, A. Gurlo, B. Klötzer, S. Penner
CrystEngComm 21 (2019) 145-154
https://doi.org/10.1039/c8ce01726c (Green OA)

Substoichiometric Zirconia Thin Films Prepared by Reactive Sputtering of Metallic Zirconium Using a Direct Current Ion Beam Source
T. Götsch, B.Neumann, B. Klötzer, S. Penner
Surface Science 680 (2019) 52-60
https://doi.org/10.1016/j.susc.2018.10.015 (Green OA)

Complex oxide thin films: Pyrochlore, defect fluorite and perovskite model systems for structural, spectroscopic and catalytic studies **P01/03**
T.Götsch, D. Hauser, N. Köpfle, J. Bernardi, B. Klötzer, S. Penner
Applied Surface Science 452 (2018) 190-200
https://doi.org/10.1016/j.apsusc.2018.05.019 (Green OA)

Zirconium-Assisted Activation of Palladium To Boost Syngas Production by Methane Dry Reforming
N. Köpfle, T. Götsch, M. Grünbacher, E. A. Carbonio, M. Hävecker, A. Knop-Gericke, L. Schlicker, A. Doran, D. Kober, A. Gurlo, S. Penner, B. Klötzer
Angew. Chem. Int. Ed. 57 (2018) 14613 –14618

https://doi.org/10.1002/anie.201807463 (Hybrid OA)

Zirconium-assistierte Aktivierung von Palladium zur Steigerung der Produktion von Synthesegas in der Trockenreformierung von Methan
N. Köpfle, T. Götsch, M. Grünbacher, E. A. Carbonio, M. Hävecker, A. Knop-Gericke, L. Schlicker, A. Doran, D. Kober, A. Gurlo, S. Penner, B. Klötzer
Angew. Chem. 130 (2018) 14823 –14828
https://doi.org/10.1002/ange.201807463 (Hybrid OA)

Visualizing catalyst heterogeneity by a multifrequential oscillating reaction **P01/02/04**
Y. Suchorski, M. Datler, I. Bespalov, J. Zeininger, M. Stöger-Pollach, J. Bernardi, H. Grönbeck, G. Rupprechter
Nature Communications 9:600 (2018) 1-6
https://doi.org/10.1038/s41467-018-03007-3 (Gold OA)

Surface composition changes of CuNi-ZrO_2 during methane decomposition: an operando NAP-XPS and density functional study **P01/02/03**
A. Wolfbeisser, G. Kovács, S. Kozlov, K. Föttinger, J. Bernardi, B. Klötzer, K.M. Neyman, G. Rupprechter
Catalysis Today 283 (2017) 134 - 143
https://doi.org/10.1016/j.cattod.2016.04.022 (Hybrid OA)

Consequences of the CMR effect on EELS in TEM **P01/09**
W. Wallisch, M. Stöger-Pollach, E. Navickas
Ultramicroscopy 179 (2017) 84 - 89
https://doi.org/10.1016/j.ultramic.2017.04.011 (No OA)

comment: open access preprint version available at arXiv.org
Synthesis and properties of monolayer-protected Cox(SC_2H_4Ph)m nanoclusters **P01/02**
S. Pollitt, E. Pittenauer, C. Rameshan, T. Schachinger, O. Safonova, V. Truttmann, B. Abhijit, G. Allmaier, N. Barrabés-Rabanal, G. Rupprechter
The Journal of Physical Chemistry C 121 (2017) 10948 - 10956
https://doi.org/10.1021/acs.jpcc.6b12076 (No OA)

Structural and catalytic properties of Ag- and Co_3O_4-Impregnated strontium titanium ferrite $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$ in methanol steam reforming **P01/03**
K. Ploner, T. Götsch, G. Kogler, R. Thalinger, J. Bernardi, Q. Zhao, C. Zhuo, B. Klötzer, S. Penner
Industrial & engineering chemistry research 56(46) (2017) 13654-13662
https://doi.org/10.1021/acs.iecr.7b03778 (Green OA)

Dislocations accelerate oxygen ion diffusion in La0.8Sr0.2MnO3 epitaxial thin films **P01/09**
E. Navickas, Y. Chen, Q. Lu, W. Wallisch, T. Huber, J. Bernardi, M. Stöger-Pollach, G. Friedbacher, H. Hutter, B. Yildiz, J. Fleig
ACS Nano 11 (2017) 11475 - 11487
https://doi.org/10.1021/acsnano.7b06228 (Hybrid OA)
A comparative discussion of the catalytic activity and CO_2-selectivity of Cu-Zr and Pd-Zr (intermetallic) compounds in methanol steam reforming **P01/03**

N. Köpfle, L. Mayr, D. Schmidmair, J. Bernardi, A. Knop-Gericke, M. Hävecker, B. Klötzer, S. Penner
Catalysts 7(2) (2017) 53
https://doi.org/10.3390/catal7020053 (Hybrid OA)

Carbon tolerance of Ni-Cu and Ni-Cu/YSZ sub-mu m sized SOFC thin film model systems **P01/03**
T. Götsch, T. Schachinger, M. Stöger-Pollach, R. Kaindl, S. Penner
Applied Surface Science 402 (2017) 1-11
https://doi.org/10.1016/j.apsusc.2017.01.076 (Green OA)

The crystallographic and electronic phase diagrams of yttria-stabilized zirconia model electrolytes **P01/03**
T. Götsch, A. Menzel, E. Bertel, M. Stöger-Pollach, S. Penner
ECS Transactions 78 (2017) 311 - 319
https://doi.org/10.1149/07801.0311ecst (No OA)

Methane dry reforming over ceria-zirconia supported Ni catalysts **P01/02**
A. Wolfbeisser, O. Sophiphun, J. Bernardi, J. Wittayakun, K. Föttinger, G. Rupprechter
Catalysis Today 277 (2016) 234 - 245
https://doi.org/10.1016/j.cattod.2016.04.025 (Hybrid OA)

Rhodium-catalyzed methanation and methane steam reforming reactions on rhodium-perovskite systems: metal-support interaction **P01/03**
R. Thalinger, T. Götsch, C. Zhuo, W. Hetaba, W. Wallisch, M. Stöger-Pollach, D. Schmidmair, B. Klötzer, S. Penner
ChemCatChem 8(12) (2016) 2057-2067
https://doi.org/10.1002/cctc.201600262 (Green OA)

Ni-perovskite interaction and its structural and catalytic consequences in methane steam reforming and methanation reactions **P01/03**
R. Thalinger, M. Gocyla, M. Heggen, R. Duhin-Borkowski, M. Grünbacher, M. Stöger-Pollach, D. Schmidmair, B. Klötzer, S. Penner
Journal of Catalysis 337 (2016) 26-35
https://doi.org/10.1016/j.jcat.2016.01.020 (Green OA)

Microstructural and chemical evolution and analysis of a self-activating CO_2-selective Cu-Zr bimetallic methanol steam reforming catalyst **P01/03**
L. Mayr, N. Köpfle, B. Klötzer, T. Götsch, J. Bernardi, S. Schwarz, T. Keilhauer, M. Armbrüster, S. Penner
Journal of Physical Chemistry 120(44) (2016) 25395-25404
https://doi.org/10.1021/acs.jpcc.6b07824 (Green OA)

Boosting hydrogen production from methanol and water by in situ activation of bimetallic Cu-Zr species **P01/03**
L. Mayr, B. Klötzer, D. Schmidmair, N. Köpfle, J. Bernardi, S. Schwarz, M. Armbrüster, S. Penner

ChemCatChem 8(10) (2016) 1778-1781
https://doi.org/10.1002/cctc.201600361 (Green OA)

Operando XAS and NAP-XPS studies of preferential CO oxidation on Co_3O_4 and CeO_2-Co_3O_4 catalysts **P01/02**
L. Lukashuk, K. Föttinger, E. Kolar, C. Rameshan, D. Teschner, M. Hävecker, A. Knop-Gericke, N. Yigit, H. Li, E. McDermott, M. Stöger-Pollach, G. Rupprechter
Journal of Catalysis 344 (2016) 1 - 15
https://doi.org/10.1016/j.jcat.2016.09.002 (Hybrid OA)

Distinct carbon growth mechanisms on the components of Ni/YSZ materials **P01/03**
M. Kogler, E. M. Köck, M. Stöger-Pollach, S. Schwarz, T. Schachinger, B. Klötzer, S. Penner
Materials Chemistry and Physics 173 (2016) 508-515
https://doi.org/10.1016/j.matchemphys.2016.02.046 (Green OA)

High-temperature carbon deposition on oxide surfaces by CO disproportionation **P01/03**
M. Kogler, E. M. Köck, B. Klötzer, T. Schachinger, W. Wallisch, R. Henn, C. W. Huck, C. Hejny, S. Penner
Journal of Physical Chemistry C 120(3) (2016) 1795-1807
https://doi.org/10.1021/acs.jpcc.5b12210 (Hybrid OA)

From zirconia to yttria: Sampling the YSZ phase diagram using sputter-deposited thin films **P01/03**
T. Götsch, W. Wallisch, M. Stöger-Pollach, B. Klötzer, S. Penner
AIP Advances 6(2) (2016) 025119
https://doi.org/10.1063/1.4942818 (Gold OA)

Hydrogen oxidation on stepped Rh surfaces: µm-scale versus nanoscale **P01/02/04**
M. Datler, I. Bespalov, S. Buhr, J. Zeininger, M. Stöger-Pollach, J. Bernardi, G. Rupprechter, Y. Suchorski
Catalysis Letters 146 (2016) 1867 - 1874
https://doi.org/10.1007/s10562-016-1824-4 (Hybrid OA)

Surface spectroscopy on UHV-grown and technological Ni-ZrO_2 reforming catalysts: from UHV to operando conditions **P01/02**
K. Anic, A. Wolfbeisser, H. Li, C. Rameshan, K. Föttinger, J. Bernardi, G. Rupprechter
Topics in Catalysis 59 (2016) 1614 - 1627
https://doi.org/10.1007/s11244-016-0678-8 (Hybrid OA)

Different synthesis protocols for Co_3O_4-CeO_2 catalysts. part 1: influence on the morphology on the nanoscale **P01/02/10**
J. Yang, L. Lukashuk, J. Akbarzadeh, M. Stöger-Pollach, H. Peterlik, K. Föttinger, G. Rupprechter, U. Schubert
Chemistry - A European Journal 21 (2015) 885 - 892
https://doi.org/10.1002/chem.201403636 (Hybrid OA)

Surface modification processes during methane decomposition on Cu-promoted Ni-ZrO_2 catalysts **P01/02**

A. Wolfbeisser, B. Klötzer, L. Mayr, R. Rameshan, D. Zemlyanov, J. Bernardi, K. Föttinger, G. Rupprechter
Catalysis Science & Technology 5 (2015) 967 - 978
https://doi.org/10.1039/C4CY00988F (Hybrid OA)

Fast oxygen exchange and diffusion kinetics of grain boundaries in Sr-doped $LaMnO_3$ thin films **P01/09**
E. Navickas, T. Huber, Y. Chen, W. Hetaba, G. Holzlechner, G. M. Rupp, M. Stöger-Pollach, G. Friedbacher, H. Hutter, B. Yildiz, J. Fleig
Physical Chemistry Chemical Physics 17 (2015) 7659 - 7669
https://doi.org/10.1039/c4cp05421k (Hybrid OA)

Preparation and characterization of epitaxially grown unsupported yttria-stabilized zirconia (YSZ) thin films **P01/03**
T. Götsch, L. Mayr, M. Stöger-Pollach, B. Klötzer, S. Penner
Applied Surface Science 331 (2015) 427-436
https://doi.org/10.1016/j.apsusc.2015.01.068 (Green OA)

Correlating surface cation composition and thin film microstructure with the electrochemical performance of lanthanum strontium cobaltite (lsc) electrodes **P01/09**
G. M. Rupp, A. Limbeck, M. Kubicek, A. Penn, M. Stöger-Pollach, G. Friedbacher, J. Fleig
Journal of Materials Chemistry A 2 (2014) 7099 - 7108
https://doi.org/10.1039/c3ta15327d (Hybrid OA)

Metal-support interaction in Pt/VO_x and Pd/VO_x systems: A comparative (HR)TEM study **P01/03**
S. Penner, M. Stöger-Pollach, R. Thalinger
Catalysis Letters 144(1) (2014) 87-96
https://doi.org/10.1007/s10562-013-1095-2 (No OA)

Cation diffusion in $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ below 800 °C and its relevance for Sr segregation **P01/09**
M. Kubicek, G. M. Rupp, S. Huber, A. Penn, A.K. Opitz, J. Bernardi, M. Stöger-Pollach, H. Hutter, J. Fleig
Physical Chemistry Chemical Physics 16 (2014) 2715 - 2726
https://doi.org/10.1039/c3cp51906f (Green OA)

Electrochemical properties of $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ thin films investigated by complementary impedance spectroscopy and isotope exchange depth profiling **P01/09**
M. Kubicek, T. Huber, A. Wachter-Welzl, A. Penn, G. M. Rupp, J. Bernardi, M. Stöger-Pollach, H. Hutter, J. Fleig
Solid State Ionics 256 (2014) 38 - 44
https://doi.org/10.1016/j.ssi.2013.12.016 (Hybrid OA)

Enhanced kinetic stability of pure and Y-doped tetragonal ZrO_2 **P01/03**
M. Kogler, E. M. Köck, S. Vanicek, D. Schmidmair, T. Götsch, M. Stöger-Pollach, C. Hejny, B. Klötzer, S. Penner
Inorganic Chemistry 53(24) (2014) 13247-13257
https://doi.org/10.1021/ic502623t (No OA)

Methane decomposition and carbon growth on Y_2O_3, yttria-stabilized zirconia and ZrO_2 **P01/03**
M. Kogler, E. M. Köck, L. Perfler, T. Bielz, M. Stöger-Pollach, W. Hetaba, M. Willinger, X. Huang, M. Schuster, B. Klötzer, S. Penner
Chemistry of Materials 26(4) (2014) 1690-1701
https://doi.org/10.1021/cm404062r (Hybrid OA)

The nanoscale kirkendall effect in Pd-based intermetallic phases **P01/03**
T. Götsch, M. Stöger-Pollach, R. Thalinger, S. Penner
Journal of Physical Chemistry C 118(31) (2014) 17810-17818
https://doi.org/10.1021/jp505458v (No OA)

The role of defects in the local reaction kinetics of CO oxidation on low-index Pd surfaces **P01/02/04/05**
D. Vogel, C. Spiel, M. Schmid, M. Stöger-Pollach, R. Schlögl, Y. Suchorski, G. Rupprechter
Journal of Physical Chemistry C 117 (2013) 12054 - 12060
https://doi.org/10.1021/jp312510d (Hybrid OA)

Thin film model systems of ZrO_2 and Y_2O_3 as templates for potential industrial applications investigated by means of electron microscopy **P01/03**
R. Thalinger, M. Stöger-Pollach, B. Klötzer, S. Penner
Materials Chemistry and Physics 138 (2013) 384 - 391
https://doi.org/10.1016/j.matchemphys.2012.11.071 (No OA)

Electron microscopy investigations of metal-support interaction effects in M/Y_2O_3 and M/ZrO_2 thin films (M=Cu, Ni) **P01/03**
R. Thalinger, M. Stöger-Pollach, W. Hetaba, M. Feuerbacher, B. Klötzer, S. Penner
Materials Chemistry and Physics 143 (2013) 167 - 177
https://doi.org/10.1016/j.matchemphys.2013.08.048 (No OA)

Formation and stability of small well-defined Cu- and Ni oxide particles **P01/03**
R. Thalinger, M. Heggen, D.G. Stroppa, M. Stöger-Pollach, B. Klötzer, S. Penner
Materials Chemistry and Physics 143 (2013) 184 - 194
https://doi.org/10.1016/j.matchemphys.2013.08.050 (No OA)

Conductive AFM and chemical analysis of highly conductive paths in dc degraded PZT with Ag/Pd electrodes P01/09
L. Andrejs, H. Oßmer, G. Friedbacher, J. Bernardi, A. Limbeck, J. Fleig
Solid State Ionics 244 (2013) 5 - 16
https://doi.org/10.1016/j.ssi.2013.04.020 (No OA)

$La_{0.6}Sr_{0.4}CoO_{3-\delta}$ (lsc) thin film electrodes with very fast oxygen reduction kinetics prepared by a solgel route **P01/09**
J. Januschewsky, M. Stöger-Pollach, F. Kubel, G. Friedbacher, J. Fleig
Zeitschrift für Physikalische Chemie 226 (2012) 889 - 899
https://doi.org/10.1524/zpch.2012.0278 (No OA)

Project Part 02 G. Rupprechter

CO oxidation on stepped Rh surfaces: µm-scale versus nanoscale **P02/04**
Y. Suchorski, I. Bespalov, J. Zeininger, M. Raab, M. Datler, P. Winkler, G. Rupprechter
Catalysis Letters, online published
https://doi.org/10.1007/s10562-019-02950-0 (Hybrid OA)

A modeling analysis of molecular orientation at interfaces by polarization-dependent sum frequency generation vibrational spectroscopy
X. Li, G. Rupprechter
Chinese Journal of Catalysis 40 (2019) 1655–1667
https://doi.org/10.1016/S1872-2067(19)63357-7 (planned Green OA)

Operando XAS and NAP-XPS investigation of CO oxidation on meso- and nanoscale CoO catalysts **P01/02**
L. Lukashuk, N. Yigit, H. Li, J. Bernardi, K. Föttinger, G. Rupprechter
Catalysis Today 336 (2019) 139-147
https://doi.org/10.1016/j.cattod.2018.12.052 (Hybrid OA)

Surface-structure libraries: Multifrequential oscillations in catalytic hydrogen oxidation on rhodium **P01/02/04**
Y. Suchorski, M. Datler, I. Bespalov, J. Zeininger, M. Stöger-Pollach, J. Bernardi,
H. Grönbeck, G. Rupprechter
Journal of Physical Chemistry C 123 (2019) 4217-4227 (OA)
https://doi.org/10.1021/acs.jpcc.8b11421

Preface: Surface science of functional oxides **P02/07**
U. Diebold, G. Rupprechter
Surface Science Science 681 (2019) A1
https://doi.org/10.1016/j.susc.2018.11.017

Transmitting metal-oxide interaction by solitary chemical waves: H_2 oxidation on ZrO_2 supported Rh **P02/04**
Y. Suchorski, M. Datler, I. Bespalov, C. Freytag, J. Zeininger, G. Rupprechter
Surface Science 679 (2019) 163-168
https://doi.org/10.1016/j.susc.2018.08.027 (Hybrid OA)

CO_2 activation on ultrathin ZrO_2 film by H_2O co-adsorption: In situ NAP-XPS and IRAS studies
H. Li, C. Rameshan, A.V. Bukhtiyarov, I.P. Prosvirin, V.I. Bukhtiyarov,
G. Rupprechter
Surface Science 679 (2019) 139-146
https://doi.org/10.1016/j.susc.2018.08.028 (Hybrid OA)

The chemical evolution of the $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ surface under SOFC operating conditions and its implications for electrochemical oxygen exchange activity **P02/03/09**

A.K. Opitz, C. Rameshan, M. Kubicek, G.M. Rupp, A. Nenning, T. Götsch, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, B. Klötzer, J. Fleig
Topics in Catalysis 61 (2018) 2129-2124
https://doi.org/10.1007/s11244-018-1068-1 (Hybrid OA)

Heterogeneous surfaces as structure and particle size libraries of model catalysts **P02/04**
Y. Suchorski, G. Rupprechter
Catalysis Letters 148 (2018) 2947-2956
https://doi.org/10.1007/s10562-018-2506-1 (Hybrid OA)

Polykristalline Oberflächen als Strukturbibliothek für die heterogene Katalyse **P02/04**
Y. Suchorski, G. Rupprechter
Nachrichten aus der Chemie 66 (2018) 851-856
https://doi.org/10.1002/nadc.20184075554

In situ NAP-XPS spectroscopy during methane dry reforming on ZrO_2/Pt(111) inverse model catalyst
C. Rameshan, H. Li, K. Anic, M. Roiaz, V. Pramhaas, R. Rameshan, R. Blume,
M. Hävecker, R. J. Knudsen, A. Knop-Gericke, G. Rupprechter
J Phys Cond Matter 30 (2018) 264007
https://doi.org/10.1088/1361-648X/aac6ff (Hybrid OA)

The role of metal-oxide interfaces for long-range metal particle activation during CO oxidation **P02/04**
Y. Suchorski, S. M. Kozlov, I. Bespalov, M. Datler, D. Vogel, Z. Budinska,
K. M. Neyman, G. Rupprechter
Nature Materials (2018)
https://doi.org/10.1038/s41563-018-0080-y (No OA, Green OA planned)
Press release: https://www.tuwien.ac.at/en/news/news_detail/article/125833/

Polarization-dependent SFG spectroscopy of near ambient pressure CO adsorption on Pt(111) and Pd(111) revisited
X. Li, M. Roiaz, V. Pramhaas, C. Rameshan, G. Rupprechter
Topics in Catalysis 61 (2018) 751-762
https://doi.org/10.1007/s11244-018-0949-7 (Hybrid OA)

Atmospheric pressure reaction cell for operando sum frequency generation spectroscopy of ultrahigh vacuum grown model catalysts
M. Roiaz, V. Pramhaas, X. Li, C. Rameshan, G. Rupprechter
Review of Scientific Instruments 89 045104 (2018)
https://doi.org/10.1063/1.5021641 (Hybrid OA)

Visualizing catalyst heterogeneity by a multifrequential oscillating reaction **P01/02/04**
Y. Suchorski, M. Datler, I. Bespalov, J. Zeininger, M. Stöger-Pollach, J. Bernardi,
H. Grönbeck, G. Rupprechter
Nature Communications 9 (2018) 1-6
https://doi.org/10.1038/s41467-018-03007-3 (Gold OA)
Press release: https://www.tuwien.ac.at/en/news/news_detail/article/125613/

Surface science approach to Pt/carbon model catalysts: XPS, STM and microreactor studies
A.M. Motin, T. Haunold, A. Bukhtiyarov, A. Bera, C. Rameshan, G. Rupprechter
Applied Surface Science 440 (2018) 680-687
https://doi.org/10.1016/j.apsusc.2018.01.148 (Hybrid OA)

Adsorption and reaction of CO on (Pd-)Al_2O_3 and (Pd-)ZrO_2: Vibrational spectroscopy of carbonate formation
K. Föttinger, W. Emhofer, D. Lennon, G. Rupprechter
Topics in Catalysis invited 60 (2017) 1722-1734
https://doi.org/10.1007/s11244-017-0852-7 (Hybrid OA)

Surface chemistry of perovskite-type electrodes during high temperature CO_2 electrolysis investigated by operando photoelectron spectroscopy **P02/03/09**
A. K. Opitz, A. Nenning, C. Rameshan, M. Kubicek, T. Götsch, R. Blume,
M. Hävecker, A. Knop-Gericke, G. Rupprechter, B. Klötzer, J. Fleig
ACS Applied Materials & Interfaces 9 (2017) 35847-35860
https://doi.org/10.1021/acsami.7b10673 (Hybrid OA)

Surface composition changes of CuNi-ZrO_2 during methane decomposition: An operando NAPXPS and density functional study **P01/02/03**
A. Wolfbeisser, G. Kovács, S. M. Kozlov, K. Föttinger, J. Bernardi, B. Klötzer,
K. M. Neyman, G. Rupprechter
Catalysis Today 283 (2017) 134-143
https://doi.org/10.1016/j.cattod.2016.04.022 (Hybrid OA)

Hydrogen oxidation on stepped Rh surfaces: µm-scale versus nanoscale **P01/02/04**
M. Datler, I. Bespalov, S. Buhr, J. Zeininger, M. Stöger-Pollach, J. Bernardi,
G. Rupprechter, Y. Suchorski
Catalysis Letters 146 (2016) 1867-1874
https://doi.org/10.1007/s10562-016-1824-4 (Hybrid OA)

Methane dry reforming over ceria-zirconia supported Ni catalysts**P01/02**
A. Wolfbeisser, O. Sophiphun, J. Bernardi, J. Wittayakun, K. Föttinger, G. Rupprechter
Catalysis Today 277 (2016) 234-245
https://doi.org/10.1016/j.cattod.2016.04.025 (Hybrid OA)

Surface spectroscopy on UHV-grown and technological Ni-ZrO_2 reforming catalysts: from UHV to operando conditions **P01/02**
K. Anic, A.O, H. Li, C. Rameshan, K. Föttinger, J. Bernardi, G. Rupprechter
Topics in Catalysis 59 (17) (2016) 1614-1627
https://doi.org/10.1007/s11244-016-0678-8 (Hybrid OA)

Ambient pressure XPS study of mixed conducting perovskite-type SOFC cathode and anode materials under well-defined electrochemical polarization **P02/03/09**
A. Nenning, A. K. Opitz, C. Rameshan, R. Rameshan, R. Blume, M. Hävecker,
A. Knop-Gericke, G. Rupprechter, B. Klötzer, J. Fleig
The Journal of Physical Chemistry C 120 (2016) 1461-1471
https://doi.org/10.1021/acs.jpcc.5b08596 (Hybrid OA)

Local reaction kinetics by imaging **P02/04**
Y. Suchorski, G. Rupprechter
Surface Science 643 (2016) 52-58
https://doi.org/10.1016/j.susc.2015.05.021 (Hybrid OA)

Ni–CeO_2–ZrO_2 catalysts for water gas shift reaction: effect of CeO_2 contents and reduction temperature
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Water Splitting on Model-Composite La0.6Sr0.4FeO3-δ (LSF) Electrodes in H_2/H_2O Atmosphere **P02/03/09**
A.K. Opitz, A. Nenning, S. Kogler, C. Rameshan, R. Rameshan, R. Blume,
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Spatially coupled catalytic ignition of CO oxidation on Pt: Mesoscopic versus nano-scale **P02/04**
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Initial stages of oxide formation on the Zr surface at low oxygen pressure: an in situ FIM and XPS study **P02/04**
I. Bespalov, M. Datler, S. Buhr, W. Drachsel, G. Rupprechter, Y. Suchorski*
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Analysing the reaction kinetics for individual catalytically active components: CO oxidation on a Pd powder supported by Pt foil **P02/04**
M. Datler, I. Bespalov, G. Rupprechter, Y. Suchorski*
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M. Datler, I. Bespalov, G. Rupprechter, Y. Suchorski*
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The growth of an ultrathin zirconia film on Pt3Zr examined by-HR-XPS, TPD, STM and DFT **P02/05/11**
H. Li, J.J. Choi, W. Mayr-Schmölzer, C. Weilach, C. Rameshan, F. Mittendorfer,
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Beschleunigung der elektrochemischen Wasserspaltungskinetik durch polarisations-getriebene Bildung von oberflächennahem Eisen(0): Eine in-situ XPS Studie an Perowskit-Elektroden **P02/03/09**
K. Opitz, A. Nenning, C. Rameshan, R. Rameshan, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, J. Fleig, B. Klötzer
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Enhancing electrochemical water-splitting kinetics by polarization-driven formation of nearsurface Fe0: an in-situ XPS study on perovskite-type electrodes **P02/03/09**
A. K. Opitz, A. Nenning, C. Rameshan, R. Rameshan, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, J. Fleig, B. Klötzer
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Surface modification during methane decomposition on Cu-promoted Ni-ZrO_2 catalysts **P01/02/03**
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Different synthesis protocols for Co_3O_4-CeO_2 catalysts. Part 1: Influence on the morphology on the nanoscale **P01/02/10**
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High surface area ceria for CO oxidation prepared from cerium t-butoxide by combined sol-gel and solvothermal processing **P02/10**
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Mapping the local reaction kinetics by PEEM: CO oxidation on individual (100)-type grains of Pt foil **P02/04**
D. Vogel, C. Spiel, Y. Suchorski, A. Urich, R. Schlögl, G. Rupprechter
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Catalytic CO oxidation on individual (110) domains of a polycrystalline Pt foil: Local reaction kinetics by PEEM **P02/04**
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Project Part 03 B. Klötzer

Crystallographic and electronic evolution of lanthanum strontium ferrite ($La_{0.6}Sr_{0.4}FeO_{3-\delta}$) thin film and bulk model systems during iron exsolution **P01/03**
T. Götsch, N. Köpfle, M. Grünbacher, J. Bernardi, E. A. Carbonio, M. Hävecker, A. Knop-Gericke, M. F. Bekheet, L. Schlicker, A. Doran, A. Gurlo, A. Franz, B. Klötzer, S. Penner
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Complex oxide thin films: Pyrochlore, defect fluorite and perovskite model systems for structural, spectroscopic and catalytic studies **P01/03**
T.Götsch, D. Hauser, N. Köpfle, J. Bernardi, B. Klötzer, S. Penner
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Role of precursor carbides for graphene growth on Ni(111) **P03/06/11**
R. Rameshan, V. Vonk, D. Franz, J. Drnec, S. Penner, A. Garhofer, F. Mittendorfer, A. Stierle, B. Klötzer
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CO_2 reduction on the pre-reduced mixed ionic-electronic conducting perovskites $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ and $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$ **P03/09**
M. Grünbacher, T. Götsch, A. K. Opitz, B. Klötzer, S. Penner
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Structural investigations of $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ under reducing conditions: kinetic and thermodynamic limitations for phase transformations and iron exsolution phenomena
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Structural and catalytic properties of Ag- and Co_3O_4-impregnated strontium sitanium ferrite $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$ in methanol steam reforming **P01/03**
K. Ploner, T. Götsch, G. Kogler, R. Thalinger, J. Bernardi, Q. Zhao, C. Zhuo, B. Klötzer, S. Penner
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Surface chemistry of perovskite-type electrodes during high temperature CO_2 electrolysis investigated by operando photoelectron spectroscopy **P02/03/09**

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Carbon tolerance of Ni-Cu and Ni-Cu/YSZ sub-µ sized SOFC thin film model systems **P01/03**
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Surface chemistry of pure tetragonal ZrO2 and gas-phase dependence of the tetragonal-to-monoclinic ZrO_2 transformation **P02/03**
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Surface composition changes of CuNi-ZrO2 during methane decomposition: An operando NAP-XPS and density functional study **P01/02/03**
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A comparative discussion of the catalytic activity and CO2-selectivity of Cu-Zr and Pd-Zr (intermetallic) compounds in methanol steam reforming **P01/03**
N. Köpfle, L. Mayr, D. Schmidmair, J. Bernardi, A. Knop-Gericke, M. Hävecker, B. Klötzer,S. Penner
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Microstructural and chemical evolution and analysis of a self-activating CO_2-selective Cu-Zr bimetallic methanol steam reforming catalyst **P01/03**
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Evidence for dissolved hydrogen in the mixed ionic-electronic conducting perovskites $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ and $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$
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Structure-property relationships in the Y_2O_3-ZrO_2 phase diagram: Influence of the Y-content on reactivity in C1 gases, surface conduction, and surface chemistry
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Metastable corundum-type In_2O_3: Phase stability, reduction properties, and catalytic characterization
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Distinct carbon growth mechanisms on the components of Ni/YSZ materials **P01/03**
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From zirconia to yttria: Sampling the YSZ phase diagram using sputter-deposited thin films **P01/03**
T. Götsch, W. Wallisch, M. Stöger-Pollach, B. Klötzer, S. Penner
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Ambient pressure XPS study of mixed conducting perovskite-type SOFC cathode and anode materials under well-defined electrochemical polarization **P02/03/09**
A. Nenning, A. K. Opitz, C. Rameshan, R. Rameshan, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, B. Klötzer, J. Fleig
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High-temperature carbon deposition on oxide surfaces by CO disproportionation **P01/03**
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Near-ambient-pressure X-ray photoelectron spectroscopy study of methane-induced carbon deposition on clean and copper-modified polycrystalline nickel materials
R. Rameshan, L. Mayr, B. Klötzer, D. Eder, A. Knop-Gericke, M. Hävecker, R. Blume, R. Schlögl, D. Zemlyanov, S. Penner

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Exsolution of Fe and SrO nanorods and nanoparticles from lanthanum strontium ferrite $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ materials by hydrogen reduction
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Trimethylaluminum and oxygen atomic layer deposition on hydroxyl-free Cu(111)
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Water-gas shift and methane reactivity on reducible perovskite-type oxides **P03/09**
R. Thalinger, A. K. Opitz, S. Kogler, M. Heggen, D. Stroppa, D. Schmidmair, R. Tappert, J. Fleig, B. Klötzer, S. Penner
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Preparation and characterization of epitaxially grown unsupported yttria-stabilized zirconia (YSZ) thin films **P01/03**
T. Götsch, L. Mayr, M. Stöger-Pollach, B. Klötzer, S. Penner
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Formation of intermetallic compounds by reactive metal support interaction: A frequently encountered phenomenon in catalysis
S. Penner, M. Armbrüster
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Enhancing electrochemical water-splitting kinetics by polarization-driven formation of nearsurface iron(0): An in situ XPS study on perovskite-type electrodes **P02/03/09**
A. K. Opitz, A. Nenning, C. Rameshan, R. Rameshan, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, J. Fleig, B. Klötzer
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Surface modification processes during methane decomposition on Cu-promoted Ni-ZrO_2 catalysts **P02/03**
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Steering of methanol reforming selectivity by zirconia-copper interaction
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Enhanced kinetic stability of pure and Y-doped tetragonal ZrO_2 **P01/03**
M. Kogler, E. M. Köck, S. Vanicek, D. Schmidmair, T. Götsch, M. Stöger-Pollach, C. Hejny, B. Klötzer, S. Penner
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The nanoscale kirkendall effect in Pd-based intermetallic phases **P01/03**
T. Götsch, M. Stöger-Pollach, R. Thalinger, S. Penner
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A high-temperature, ambient-pressure ultra-dry operando reactor cell for fourier-transform infrared spectroscopy
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Pure and mixed-oxide thin film model systems grown on sodium chloride templates for structural and catalytic studies
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Metal-support interaction in Pt/VOx and Pd/VOx systems: A comparative (HR)TEM study **P01/03**
S. Penner, M. Stöger-Pollach, R. Thalinger
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Combined UHV/high-pressure catalysis setup for depth-resolved near-surface spectroscopic characterization and catalytic testing of model catalysts
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Hydrogen surface reactions and adsorption studied on Y_2O_3, YSZ, and ZrO_2
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Methane decomposition and carbon growth on Y_2O_3, yttria-stabilized zirconia and ZrO_2 **P01/03**
M. Kogler, E. M. Köck, L. Perfler, T. Bielz, M. Stöger-Pollach, W. Hetaba, M. Willinger, X. Huang, M. Schuster, B. Klötzer, S. Penner
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Electron microscopy investigations of metal-support interaction effects in M/Y_2O_3 and M/ZrO_2 thin films (M=Cu, Ni) **P01/03**
R. Thalinger, M. Stöger-Pollach, W. Hetaba, M. Feuerbacher, B. Klötzer, S. Penner
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Formation and stability of small well-defined Cu- and Ni oxide particles **P01/03**
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Thin film model systems of ZrO_2 and $Y2O_3$ as templates for potential industrial applications investigated by means of electron microscopy **P01/03**
R. Thalinger, M. Stöger-Pollach, B. Klötzer, S. Penner
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Project Part 04 Y. Suchorski

Surface-Structure Libraries: Multifrequential Oscillations in Catalytic Hydrogen Oxidation on Rhodium **P01/04**
Y. Suchorski, M. Datler, I. Bespalov, J. Zeininger, M. Stöger-Pollach, J. Bernardi, H. Grönbeck, G. Rupprechter
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Transmitting metal-oxide interaction by solitary chemical waves: H_2 oxidation on ZrO_2 supported Rh **P02/04**
Y. Suchorski, M. Datler, I. Bespalov, C. Freytag, J. Zeininger, G. Rupprechter
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Polykristalline Oberflächen als Strukturbibliothek für die heterogene Katalyse **P02/04**
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Hydrogen oxidation on stepped Rh surfaces: µm-scale versus nanoscale **P01/02/04**
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Spatially coupled catalytic ignition of CO oxidation on Pt: mesoscopic versus nano-scale **P02/04**
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C. Spiel, P. Blaha, Y. Suchorski, K. Schwarz, G. Rupprechter
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Catalytic CO oxidation on individual (110) domains of a polycrystalline Pt foil: Local Reaction Kinetics by PEEM **P02/04**
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Project Part 05 M. Schmid

Cation Non-stoichiometry in Oxides: Pushing Detection to its Limits **P05/07**
M. Riva, G. Franceschi, Q. Lu, M. Schmid, B. Yildiz, U. Diebold
Physical Review Materials (in press April 2019)

Incipient ferroelectricity: A route towards bulk-terminated $SrTiO_3$ (001) **P05/07**
I. Sokolovic, M. Schmid, U. Diebold, M. Setvin
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Interplay between adsorbates and polarons: CO on rutile TiO_2(110) **P05/07**
M. Reticcioli, I. Sokolovic, M. Schmid, U. Diebold, M. Setvin, C. Franchini
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Surface structures of ZrO_2 films on Rh(111): From two layers to bulk termination **P05/07**
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Adsorption of CO on the $Ca_3Ru_2O_7$(001) surface **P05/07/11**
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Water adsorption at ZrO_2: The ZrO_2(111)/Pt_3Zr(0001) model system **P03/05/07/11**
P. Lackner, J. Hulva, E.-M. Köck, W. Mayr-Schmölzer, J.I.J. Choi, S. Penner,
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High affinity adsorption leads to molecularly ordered interfaces on model TiO_2 in air and solution **P05/07**
J. Balajka, M.A. Hines, W.J.I. DeBenedetti, M. Komora, J. Pavelec, M. Schmid, U. Diebold
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Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide **P05/07/09**
M. Riva, M. Kubicek, X. Hao, G. Franceschi, S. Gerhold, M. Schmid, H. Hutter, J. Fleig, C. Franchini, B. Yildiz, U. Diebold
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Water adsorption at ZrO_2: The ZrO_2(111)/Pt_3Zr(0001) model system to powder amples **P03/05/07/11**
P. Lackner, J. Hulva, E.-M. Köck, W. Mayr-Schmölzer, J.I.J. Choi, S. Penner, U. Diebold,
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Water agglomerates on Fe_3O_4(001) **P05/07**
M. Meier, J. Hulva, Z. Jakub, J. Pavelec, M. Setvin, R. Bliem, M. Schmid, U. Diebold,
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Prototypical organic–oxide interface: intra-molecular resolution of sexiphenyl on In_2O_3(111) **P05/07**
M. Wagner, J. Hofinger, M. Setvin, L. A. Boatner, M. Schmid, U. Diebold
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A monolayer of superoxide on the $Ca_3Ru_2O_7$(001) surface **P05/07/11**
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Polarity compensation mechanism on the perovskite surface $KTaO_3$(001) **P05/07**
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Probing the geometry of copper and silver adatoms on magnetite: Quantitative experiments versus theory **P05/07**
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F. Kraushofer, Z. Jakub, M. Bichler, J. Hulva, P. Drmota, M. Weinold, M. Schmid, M. Setvin, U. Diebold, P. Blaha, G. S. Parkinson
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Construction and evaluation of an ultrahigh-vacuum-compatible sputter deposition source **P05/07**
P. Lackner, J.-I. J. Chong, U. Diebold, M. Schmid
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Zirconium-palladium interactions during dry reforming of methane **P03/05**
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Resolving the structure of a well-ordered hydroxlated overlayer on In_2O_3(111): nanomanipulation and theory **P05/07**
M. Wagner, P. Lackner, S. Seiler, A. Brunsch, R. Bliem, S. Gerhold, Z. Wang, J. Osiecki, K. Schulte, L.A. Boatner, M. Schmid, B. Meyer, U. Diebold
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Ordered hydroxyls on $Ca_3Ru_2O_7$(001) **P05/07/11**
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A multi-technique study of CO_2 adsorption on Fe_3O_4 magnetite **P05/07**
J. Pavelec, J. Hulva, D. Halwidl, R. Bliem, O. Gamba, Z. Jakub, F. Brunbauer, M. Schmid, U. Diebold, G.S. Parkinson
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The role of surface defects in the adsorption of methanol on Fe_3O_4(001) **P05/07**
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Well-ordered in adatoms at the In_2O_3(111) surface created by Fe depositon **P05/07**
M. Wagner, P. Lackner, S. Seiler, S. Gerhold, J. Osiecki, K. Schulte, L.A. Boatner, M. Schmid, B. Meyer, U. Diebold
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The dual role of CO in the stability of sub-nano Pt clusters at the Fe_3O_4(001) surface **P05/07**
R. Bliem, J. E.S. van der Hoeven, J. Hulva, J. Pavelec, O. Gamba, P. E. de Jongh, M. Schmid, P. Blaha, U. Diebold, G.S. Parkinson

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Adjusting island density and morphology of the $SrTiO_3$(110)-(4x1) surface: pulsed laser deposition combined with scanning tunneling microscopy **P05/07**
S. Gerhold, M. Riva, B. Yildiz, M. Schmid, U. Diebold
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Fe_3O_4(110)-(1x3) revisited: periodic (111) nanofacets **P05/07**
G.S. Parkinson, P. Lackner, O. Gamba, S. Maaß, S. Gerhold, M. Riva, R. Bliem, U. Diebold, M. Schmid
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Adsorption water at the SrO surface of ruthenates **P05/07/11**
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Growth of an ultrathin zirconia film on Pt_3Zr examined by high-resolution x-ray photoelectron spectroscopy, temperature-programmed desorption, scanning tunneling microscopy, and density functional theory **P02/05/11**
H. Li, J. I. J. Choi, W. Mayr-Schmölzer, C. Weilach, C. Rameshan, F. Mittendorfer, J. Redinger, M. Schmid, G. Rupprechter
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Nickel-oxide-modified $SrTiO_3$(110)-(4×1) surfaces and their interaction with water **P05/07**
S. Gerhold, M. Riva, Z. Wang, R. Bliem, M. Wagner, J. Osiecki, K. Schulte, M. Schmid, U. Diebold
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Aggregation and electronically-induced migration of oxygen vacancies in TiO_2 anatase **P05/07**
M. Setvin, M. Schmid, U. Diebold
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Coexistence of trapped and free excess electrons in $SrTiO_3$ **P05/07**
Xi. Hao, Z. Wang, M. Schmid, U. Diebold, and C. Franchini
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The growth of ultrathin zirconia films on Pd_3Zr(0001) **P05/07/11**
J.-I. J. Choi, W. Mayr-Schmölzer, F. Mittendorfer, J. Redinger, U. Diebold, M. Schmid
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Point defects at cleaved Sr n+1RunO3n+1 (001) surfaces **P05/07/11**
B. Stöger, M. Hieckel, F. Mittendorfer, Z. Wang, M. Schmid, G.S. Parkinson, D. Fobes, J. Peng, Z. Mao, J. Redinger, U. Diebold
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High chemical activity of a perovskite surface: reaction of CO with the surface of $Sr_3Ru_2O_7$ **P05/07/11**
B. Stöger, M. Hieckel, Z. Wang, F. Mittendorfer, M. Schmid, D. Fobes, J. Peng, R. Podlucky, Z. Mao, J. Redinger, U. Diebold
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Stabilizing single Ni adatoms on a two-dimensional porous titania on $SrTiO_3$(110) Surface **P05/07**
Z. Wang, X. Hao, S. Gerhold, P. Mares, M. Wagner, R. Bliem, K. Schulte, M. Schmid, C. Frachini, U. Diebold
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Vacancy clusters at domain boundaries and band bending at the $SrTiO_3$(110) surface **P05/07**
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Charge trapping at the step edges of TiO_2 anatase (101) **P05/07**
M. Setvin, X. Hao, J. Pavelec, B. Daniel, Z. Novotny, G.S. Parkinson, M. Schmid, C. Franchini, U. Diebold
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Anisotropic two-dimensional electron gas at $SrTiO_3$(110) **P05/07**
Z. Wang, Z. Zhong, X. Hao, S. Gerhold, B. Stöger, M. Schmid, J. Sanchez-Barriga, A. Varykhalov, C. Franchini, K. Held, and U. Diebold
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Stoichiometry-driven switching between surface reconstructions on $SrTiO_3$(001) **P05/07**
S. Gerhold, Z. Wang, M. Schmid, U. Diebold
Surface Science Letters 621 (2014) L1–L4
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The role of defects in the local reaction kinetics of CO oxidation on low-index Pd surfaces **P01/02/04/05**
D. Vogel, C. Spiel, M. Schmid, M. Stöger-Pollach, R. Schlögl, Y. Suchorski, G. Rupprechter
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Water adsorption at the tetrahedral titania surface layer of $SrTiO_3$(110)-(4×1) **P05/07**
Z. Wang, X. Hao, S. Gerhold, Z. Novotný,C. Franchini, E. McDermott, K. Schulte, M. Schmid, U. Diebold
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Reaction of O_2 with subsurface oxygen vacancies on TiO_2 anatase (101) **P05/07**
M. Setvin, U. Aschauer, P. Scheiber, M. Schmid, A. Selloni, U. Diebold
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(Sub)surface mobility of oxygen vacancies at the TiO_2 anatase (101) surface **P05/07**
P. Scheiber, M. Fidler, O. Dulub, M. Schmid, U. Diebold, U. Aschauer, W. Hou, A. Selloni

Physical Review Letters 109 (2012) 136103
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Pt_3Zr(0001): A substrate for growing well-ordered ultrathin zirconia films by oxidation **P05/07/11**
M. Antlanger, W. Mayer-Schmölzer, J. Pavelec, F. Mittendorfer, J. Redinger, P. Varga, U. Diebold, M. Schmid
Physical Review B 86 (2012) 035451
https://doi.org/10.1103/PhysRevB.86.035451 (Green OA)

Bulk characterization and surface properties of $In2O_3$ (100) single crystals **P05/07/09**
D. Hagleitner, P. Jacobson, S. Blomberg, K. Schulte, E. Lundgren, M. Kubicek, J- Fleig, F. Kubel, C. Puls, A. Limbeck, H. Hutter, L. A. Boatner, M. Schmid, U. Diebold
Physical Review B 85 (2012) 115441
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Project Part 06 A. Stierle

In-situ SXRD study of fuel cell model cathodes (Pu1) **P06/09**
S. Volkov, V. Vonk, T. Huber, G. Rupp, E. Navickas, T. Kubicek, V. Kilic, D. Franz, J. Fleig, A. Stierle
ESRF Beamtime Report (2014) (No OA)

Atomic structure and composition of the yttria-stabilized zirconia (111) surface
V. Vonk, N. Khorshidi , A. Stierle, H. Dosch Surface Science 612 (2013) 69–76
DOI:10.1016/j.susc.2013.02.014 (Hybrid OA)

In-situ SXRD study of fuel cell model cathodes (Pu1) **P06/09**
S. Volkov, V. Vonk, T. Huber, G. Rupp, E. Navickas, T. Kubicek, V. Kilic, D. Franz, J. Fleig, A. Stierle
ESRF Beamtime Report (2014) (No OA)

Atomic structure and composition of the yttria-stabilized zirconia (111) surface
V. Vonk, N. Khorshidi , A. Stierle, H. Dosch
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DOI:10.1016/j.susc.2013.02.014 (Hybrid OA)

Project Part 07 U. Diebold

Cation Non-stoichiometry in Oxides: Pushing Detection to its Limits **P05/07**
M. Riva, G. Franceschi, Q. Lu, M. Schmid, B. Yildiz, U. Diebold
Physical Review Materials (in press April 2019)

Incipient ferroelectricity: A route towards bulk-terminated $SrTiO_3$ (001) **P05/07**
I. Sokolovic, M. Schmid, U. Diebold, M. Setvin
Physical Review Materials 3 (2019) 034407
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Interplay between adsorbates and polarons: CO on rutile TiO_2(110) **P05/07**
M. Reticcioli, I. Sokolovic, M. Schmid, U. Diebold, M. Setvin, C. Franchini
Physical Review Letters 122 (2019) 016805
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Surface structures of ZrO_2 films on Rh(111): From two layers to bulk termination **P05/07**
P. Lackner, Z. Zou, S. Mayr, J.I.J. Choi, U. Diebold, M. Schmid
Surface Science 679 (2019) 180 - 187
https://doi.org/10.1016/j.susc.2018.09.004 (green OA)

Adsorption of CO on the $Ca_3Ru_2O_7$(001) surface **P05/07/11**
W. Mayr-Schmölzer, D. Halwidl, F. Mittendorfer, M. Schmid, U. Diebold, J. Redinger
Surface Science 680 (2019) 18-23
https://doi.org/10.1016/j.susc.2018.10.004 (green OA)

Water adsorption at ZrO_2: The ZrO_2(111)/Pt_3Zr(0001) model system **P03/05/07/11**
P. Lackner, J. Hulva, E.-M. Köck, W. Mayr-Schmölzer, J.I.J. Choi, S. Penner, U. Diebold, F. Mittendorfer, J. Redinger, B. Klötzer, G.S. Parkinson, M. Schmid
Journal of Materials Chemistry A 6 (2018) 17587
https://doi.org/10.1039/C8TA04137G (Hybrid OA)

High affinity adsorption leads to molecularly ordered interfaces on model TiO_2 in air and solution **P05/07**
J. Balajka, M.A. Hines, W.J.I. DeBenedetti, M. Komora, J. Pavelec, M. Schmid, U. Diebold
Science 361 (2018) 768-789
https://doi.org/10.1063/1.5046846

Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide **P05/07/09**
M. Riva, M. Kubicek, X. Hao, G. Franceschi, S. Gerhold, M. Schmid, H. Hutter, J. Fleig, C. Franchini, B. Yildiz, U. Diebold
Nature Communications 9 (2018) 3710
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Water adsorption at ZrO_2: The ZrO_2(111)/Pt_3Zr(0001) model system to powder amples **P03/05/07/11**
P. Lackner, J. Hulva, E.-M. Köck, W. Mayr-Schmölzer, J.I.J. Choi, S. Penner, U. Diebold, F. Mittendorfer, J. Redinger, B. Klötzer, G.S. Parkinson, M. Schmid
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Water agglomerates on Fe_3O_4(001) P05/07
M. Meier, J. Hulva, Z. Jakub, J. Pavelec, M. Setvin, R. Bliem, M. Schmid, U. Diebold,
C. Franchini, G.S. Parkinson
Proceedings of the National Academy of Sciences 115 (25) (2018) E5642-5650
https://doi.org/10.1073/pnas.1801661115 (Green OA)

Prototypical organic–oxide interface: intra-molecular resolution of sexiphenyl on In_2O_3(111) **P05/07**
M. Wagner, J. Hofinger, M. Setvin, L. A. Boatner, M. Schmid, U. Diebold
ACS Appl. Mater. Interfaces 10 (2018) 14175–14182
https://doi.org/10.1021/acsami.8b02177 (Hybrid OA)

Sexiphenyl on Cu(100)": nc-AFM tip functionalization and identification P05/07
M. Wagner, M. Setvín, M. Schmid, U. Diebold
Surface Science, in press (March 2018)
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A monolayer of superoxide on the $Ca_3Ru_2O_7$(001) surface **P05/07/11**
D. Halwidl, W. Mayr-Schmölzer, D. Fobes, J. Peng, Z. Mao, M. Setvin, M. Schmid,
F. Mittendorfer, J. Redinger, U. Diebold
Journal of Materials Chemistry A 6 (2018) 5703–5713.
https://doi.org/10.1039/C8TA00265G (Hybrid OA)

Polarity compensation mechanism on the perovskite surface $KTaO_3$(001) P05/07
M. Setvin, M. Reticcoli, F. Poeltzleitner, J. Hulva, M. Schmid, L. A. Boatner, C. Franchini, U. Diebold
Science 359 (6375), (2018) 572–575
https://doi.org/10.1126/science.aar2287 (Will be green OA after 6-month delay imposed by the publisher)

Probing the geometry of copper and silver adatoms on magnetite: Quantitative experiments versus theory **P05/07**
M. Meier, Z. Jakub, J. Balajka, J. Hulva, R. Bliem, P.K. Thakur, T. L. Lee, C. Franchini, M. Schmid, U. Diebold, F. Allegretti, D.A. Duncan, G.S. Parkinson
Nanoscale 10 (2018) 2226–2230
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Atomic-scale structure of the Fe_2O_3(1102) "r-cut" surface **P05/07**
F. Kraushofer, Z. Jakub, M. Bichler, J. Hulva, P. Drmota, M. Weinold, M. Schmid, M. Setvin, U. Diebold, P. Blaha, G. S. Parkinson
Journal of Physical Chemistry C 122 (2018) 1657–1669
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Adsorption of CO on the Fe_3O_4(001) surface **P05/07**
J. Hulva, Z. Jakub, Z. Novotný, N. Johansson, J. Knudsen, J. Schnadt, M. Schmid, U. Diebold, G.S. Parkinson
Journal of Physical Chemistry B 122 (2018) 721–729
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Resolving the structure of a well-ordered hydroxlated overlayer on In_2O_3(111): nanomanipulation and theory **P05/07**
M. Wagner, P. Lackner, S. Seiler, A. Brunsch, R. Bliem, S. Gerhold, Z. Wang, J. Osiecki, K. Schulte, L.A. Boatner, M. Schmid, B. Meyer, U. Diebold
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Surface structure of TiO2 rutile (011) exposed to liquid water **P05/07**
J. Balajka, U. Aschauer, A. Selloni, S. Mertens, M. Schmid, U. Diebold
Journal of Physical Chemisty C, 121 (2017) 26424–26431
DOI:10.1021/acs.jpcc.7b09674 (Green OA)

Construction and evaluation of an ultrahigh-vacuum-compatible sputter deposition source **P05/07**
P. Lackner, J.-I. J. Chong, U. Diebold, M. Schmid
Review of Scientific Instruments, 88 (2017) 103904
DOI:10.1063/1.4998700 (Green OA)

Methanol on anatase TiO2 (101): mechanistic insights into photocatalysis **P05/07**
M. Setvin, T. Simschitz, C. di Valentin, A. Selloni, M. Schmid, U. Diebold
ACS Catalysis, 7 (10) (2017) 7081–7091
DOI:10.1021/acscatal.7b02003 (Green OA)

Perspective article: a controversial benchmark system for water-oxide interfaces: H2O/TiO2(110)
U. Diebold
Journal of Chemical Physics, 147 (2017) 040901
DOI:10.1063/1.4996116 (Green OA)

Ordered hydroxyls on $Ca_3Ru_2O_7$(001) **P05/07/11**
D. Halwidl, W. Mayr-Schmölzer, D. Fobes, J. Peng, Z. Mao, M. Schmid, F. Mittendorfer, J. Redinger, U. Diebold
Nature Communications 8 (2017) 23
https://doi.org/10.1038/s41467-017-00066-w (Hybrid OA)

Point defects on bulk oxides, characterized by atomically-resolved scanning probe microscopy (Tutorial Review)" **P05/07**
M. Setvin, M. Wagner, M.Schmid, G.S. Parkinson, U. Diebold
Chemical Society Reviews 46 (2017) 1772 – 1784
DOI:10.1039/c7cs00076f (Green OA)

A multi-technique study of CO_2 adsorption on Fe_3O_4 magnetite **P05/07**
J. Pavelec, J. Hulva, D. Halwidl, R. Bliem, O. Gamba, Z. Jakub, F. Brunbauer, M. Schmid, U. Diebold, G.S. Parkinson
Journal of Chemical Physics 146 (2017) 014701
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The role of surface defects in the adsorption of methanol on Fe_3O_4(001) **P05/07**
O. Gamba, J. Hulva, J. Pavelec, R. Bliem, M. Schmid, U. Diebold, G.S. Parkinson
Topics in Catalysis 60 (2017) 420–430
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Well-ordered In adatoms at the In2O3(111) surface created by Fe depositon **P05/07**
M. Wagner, P. Lackner, S. Seiler, S. Gerhold, J. Osiecki, K. Schulte, L.A. Boatner, M. Schmid, B. Meyer, U. Diebold
Physical Review Letters, 117(2016) 20610
DOI:10.1103/PhysRevLett.117.206101 (Green OA)

The dual role of CO in the stability of sub-nano Pt clusters at the Fe3O4(001) surface **P05/07**
R. Bliem, J. E.S. van der Hoeven, J. Hulva, J. Pavelec, O. Gamba, P. E. de Jongh, M. Schmid, P. Blaha, U. Diebold, G.S. Parkinson
Proceedings of the National Academy of Sciences, 113 (9) (2016) 8921-8926
DOI:10.1073/pnas.1605649113 (Hybrid OA)

Metal adatoms and clusters on ultra-thin zirconia films **P05/07/11**
J.-I. J.Choi, W. Mayr-Schmölzer, I. Valenti, P. Luches, F. Mittendorfer, J. Redinger, U. Diebold, M. Schmid
Journal of Physical Chemistry C 120 (2016) 9920 – 9932
DOI:10.1021/acs.jpcc.6b03061 (Hybrid OA)

Adjusting island density and morphology of the $SrTiO_3$(110)-(4x1) surface: pulsed laser deposition combined with scanning tunneling microscopy **P05/07**
S. Gerhold, M. Riva, B. Yildiz, M. Schmid, U. Diebold
Surface Science, 651 (2016) 76–83
https://doi.org/10.1016/j.susc.2016.03.010 (Hybrid OA)

Transition from tetrahedral to octahedral coordination for high TiO2 coverages of the (110) surface of strontium titanate
Z. Wang, A. Loon, A. Subramanian, E. McDermott, J.A. Enterkin, M. Hieckel, B.C. Russell, R.J. Green, A. Moewes, J. Guo, P. Blaha, M.R. Castell, U. Diebold, L.D. Marks
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DOI:10.1021/acs.nanolett.5b05211 (Hybrid OA)

Fe_3O_4(110)-(1x3) revisited: periodic (111) nanofacets **P05/07**
G.S. Parkinson, P. Lackner, O. Gamba, S. Maaß, S. Gerhold, M. Riva, R. Bliem, U. Diebold, M. Schmid
Surface Science Letters 649 (2016) L120–L123
https://doi.org/10.1016/j.susc.2016.02.020 (Green OA)

Adsorption water at the SrO surface of ruthenates **P05/07/11**
D. Halwidl, B. Stöger, W. Mayr-Schmölzer, J. Pavelec, D. Fobes, J. Peng, Z. Mao, G.S. Parkinson, M. Schmid, F. Mittendorfer, J. Redinger, U. Diebold
Nature Materials 15 (2016) 450 – 455
https://doi.org/10.1038/nmat4512 (Green OA)

Nickel-oxide-modified $SrTiO_3$(110)-(4×1) surfaces and their interaction with water **P05/07**
S. Gerhold, M. Riva, Z. Wang, R. Bliem, M. Wagner, J. Osiecki, K. Schulte, M. Schmid, U. Diebold
Journal of Physical Chemistry C 119 (2015) 20481–20487
https://doi.org/10.1021/acs.jpcc.5b06144 (Hybrid OA)

Aggregation and electronically-induced migration of oxygen vacancies in TiO_2 anatase **P05/07**
M. Setvin, M. Schmid, U. Diebold
Physical Review B 91 (2015) 195403
https://doi.org/10.1103/PhysRevB.91.195403 (Green OA)

Coexistence of trapped and free excess electrons in $SrTiO_3$ **P05/07**
Xi. Hao, Z. Wang, M. Schmid, U. Diebold, and C. Franchini
Physical Review B 91 (2015) 085204
https://doi.org/10.1103/PhysRevB.91.085204 (Green OA)´

Point defects at cleaved Sr n+1RunO3n+1 (001) surfaces **P05/07/11**
B. Stöger, M. Hieckel, F. Mittendorfer, Z. Wang, M. Schmid, G.S. Parkinson, D. Fobes, J. Peng, Z. Mao, J. Redinger, U. Diebold
Physical Review B 90 (2014) 165438
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High chemical activity of a perovskite surface: reaction of CO with the surface of $Sr_3Ru_2O_7$ **P05/07/11**
B. Stöger, M. Hieckel, Z. Wang, F. Mittendorfer, M. Schmid, D. Fobes, J. Peng, R. Podlucky, Z. Mao, J. Redinger, U. Diebold
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Stabilizing single Ni adatoms on a two-dimensional porous titania on $SrTiO_3$(110) Surface **P05/07**
Z. Wang, X. Hao, S. Gerhold, P. Mares, M. Wagner, R. Bliem, K. Schulte, M. Schmid, C. Frachini, U. Diebold
Journal of Physical Chemistry C 118 (34) 2014, 19904–19909
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Vacancy clusters at domain boundaries and band bending at the $SrTiO_3$(110) surface **P05/07**
Z. Wang, X. Hao, S. Gerhold, M. Schmid, C. Franchini, U. Diebold
Physical Review B 90 (2014) 035436
https://doi.org/10.1103/PhysRevB.90.035436 (Hybrid OA)

The growth of ultrathin zirconia films on Pd3Zr(0001) **P05/07/11**
J.-I. J. Choi, W. Mayr-Schmölzer, F. Mittendorfer, J. Redinger, U. Diebold, M. Schmid
Journal of Physics: Condensed Matter, 26 (2014) 225003
DOI:10.1088/0953-8984/26/22/225003 (Hybrid OA)

Charge trapping at the step edges of TiO2 anatase (101) **P05/07**
M. Setvin, X. Hao, J. Pavelec, B. Daniel, Z. Novotny, G.S. Parkinson, M. Schmid, C. Franchini, U. Diebold
Angewandte Chemie, International Edition, 53 (2014) 4714 – 4716
DOI:10.1002/anie.201309796 (Green OA)

Anisotropic two-dimensional electron gas at SrTiO3(110) **P05/07**
Z. Wang, Z. Zhong, X. Hao, S. Gerhold, B. Stöger, M. Schmid, J. Sanchez-Barriga, A. Varykhalov, C. Franchini, K. Held, U. Diebold
Proceedings of the National Academy of Sciences, 111 (2014) 3933 – 3937
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Stoichiometry-driven switching between surface reconstructions on $SrTiO_3$(001) **P05/07**
S. Gerhold, Z. Wang, M. Schmid, U. Diebold
Surface Science Letters 621 (2014) L1–L4
https://doi.org/10.1016/j.susc.2013.10.015 (Hybrid OA)

Water adsorption at the tetrahedral titania surface layer of $SrTiO_3$(110)-(4×1) **P05/07**
Z. Wang, X. Hao, S. Gerhold, Z. Novotný,C. Franchini, E. McDermott, K. Schulte, M. Schmid, U. Diebold
Journal of Physical Chemistry C 117 (49) (2013) 26060–26069
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Reaction of O_2 with subsurface oxygen vacancies on TiO_2 anatase (101) **P05/07**
M. Setvin, U. Aschauer, P. Scheiber, M. Schmid, A. Selloni, U. Diebold
Science 341 (2013) 988
https://doi.org/10.1126/science.1239879 (Green OA)

Strain-mediated defect superstructure on the SrTiO3(110) surface **P05/07**
Z. Wang, F. Li, S. Meng, J. Zhang, E. W. Plummer, U. Diebold, J. Guo
Physical Review Letters 111 (2013) 056101
DOI:10.1103/PhysRevLett.111.056101 (Green OA)

(Sub)surface mobility of oxygen vacancies at the TiO_2 anatase (101) surface **P05/07**
P. Scheiber, M. Fidler, O. Dulub, M. Schmid, U. Diebold, U. Aschauer, W. Hou, A. Selloni
Physical Review Letters 109 (2012) 136103
https://doi.org/10.1103/PhysRevLett.109.136103 (Green OA)

Pt_3Zr(0001): A substrate for growing well-ordered ultrathin zirconia films by oxidation **P05/07/11**
M. Antlanger, W. Mayer-Schmölzer, J. Pavelec, F. Mittendorfer, J. Redinger, P. Varga, U. Diebold, M. Schmid
Physical Review B 86 (2012) 035451
https://doi.org/10.1103/PhysRevB.86.035451 (Green OA)

Bulk characterization and surface properties of $In2O_3$ (100) single crystals **P05/07/09**
D. Hagleitner, P. Jacobson, S. Blomberg, K. Schulte, E. Lundgren, M. Kubicek, J- Fleig, F. Kubel, C. Puls, A. Limbeck, H. Hutter, L. A. Boatner, M. Schmid, U. Diebold
Physical Review B 85 (2012) 115441
https://doi.org/10.1103/PhysRevB.85.115441 (Green OA)

Project Part 09 J. Fleig

Nano-scale oxide formation inside electrochemically formed Pt blisters at a solid electrolyte interface **P01/09**
T. F. Keller, S. Volkov, E. Navickas, S. Kulkarni, V. Vonk, J. Fleig and A. Stierle
Solid State Ionics 330 (2019) 17-23
https://doi.org/10.1016/j.ssi.2018.11.009 (Hybrid OA)

Electrochemical XPS investigation of metal exsolution on SOFC electrodes: Controlling the electrode oxygen partial pressure in ultra-high-vacuum
A. Nenning, J. Fleig
Surface Science 680 (2019) 43-51
https://doi.org/10.1016/j.susc.2018.10.006 (Hybrid OA)

The chemical evolution of the $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ surface under SOFC operating conditions and its implications for electrochemical oxygen exchange activity **P02/03/09**
A. K. Opitz, C. Rameshan, M. Kubicek, G.M. Rupp, A. Nenning, T. Götsch, R.Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, A. Klötzer, J. Fleig
Topics in Catalysis 61 (2018) 2129-2141
https://doi.org/10.1007/s11244-018-1068-1 (Hybrid OA)

Influence of surface atomic structure demonstrated on oxygen incorporation mechanism at a model perovskite oxide **P02/03/09**
M. Riva, M. Kubicek, X. Hao, S. Gerhold, G. Franceschi, M. Schmid, H. Hutter, J. Fleig, C. Franchini, B. Yildiz, U. Diebold
Nature Communications 9 (2018) 3809, p. 1-9
https://doi.org/10.1038/s41467-018-05685-5 (Gold OA)

In situ impedance analysis of oxygen exchange on growing $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ thin films,
G. M. Rupp, A.K. Opitz, M. Kubicek, J. Fleig
ACS Applied Energy Materials 1 (2018) 4522-4535
https://doi.10.1021/acsaem.8b00586 (Hybrid OA)

How to get mechanistic information from partial pressure-dependent current-voltage measurements of oxygen exchange on mixed conducting electrodes
A. Schmid, G. M. Rupp, J. Fleig
Chem. Mat. 30 (2018) 4242-4252
https://doi.org/10.1021/acs.chemmater.8b00597 (Hybrid OA)

Interplay of grain size dependent electronic and ionic conductivity in electrochemical polarization studies on Sr-doped $LaMnO_3$ (LSM) thin film cathodes
T. Huber, E. Navickas, K. Sasaki, B. Yildiz, H. Hutter, H. Tuller, J. Fleig
J. Electrochem. Soc. 165 (2018) F702-F709
https://doi.org/10.1149/2.1081809jes (Hybrid OA)

Voltage and partial pressure dependent defect chemistry of (La,Sr)$FeO_{3-\delta}$ thin films investigated by chemical capacitance measurements
A. Schmid, G. M. Rupp, J. Fleig
Phys. Chem. Chem. Phys. 20 (2018) 12016-12026
https://doi.org/10.1039/C7CP07845E (Hybrid OA)

Dislocations accelerate oxygen ion diffusion in $La_{0.8}Sr_{0.2}MnO_3$ epitaxial thin films **P01/09**
E. Navickas, Y. Chen, Q. Lu, W. Wallisch, T. M. Huber, J. Bernardi, M. Stöger-Pollach, H. Hutter, B. Yildiz, J. Fleig
ACS Nano 11 (2017) 11475-11487
https://doi.org/10.1021/acsnano.7b06228 (Hybrid OA)

The surface chemistry of perovskite-type electrodes during high temperature CO_2 electrolysis investigated by operando photoelectron spectroscopy **P02/03/09**
A.K. Opitz, A. Nenning, C. Rameshan, M. Kubicek, T. Götsch, R. Blume, M. Hävecker, A. Knop-Gericke, G. Rupprechter, B. Klötzer, J. Fleig
ACS Applied Materials and Interfaces 9 (2017) 35847–35860
https://doi.org/10.1021/acsami.7b10673 (Hybrid OA)

Revisiting the temperature dependent ionic conductivity of yttria stabilized zirconia (YSZ)
C. Ahamer, A. K. Opitz, G. M. Rupp, J. Fleig
J. Electrochem. Soc. 164 (2017) F790-F803
https://doi.org/10.1149/2.0641707jes (Hybrid OA)

Towards an improved understanding of electrochemical oxygen exchange reactions on mixed conducting oxides
J. Fleig, G. M. Rupp, A. Nenning, A. Schmid
ECS Transactions 77 (10) (2017) 93-108
https://doi.org/10.1149/07710.0093ecst (No OA)

Experimental design for voltage driven tracer incorporation and diffusion studies in oxide thin film electrodes
T.M. Huber, E. Navickas, K. Sasaki, B. Yildiz, H. Tuller, G. Friedbacher, H. Hutter, J. Fleig
J. Electrochem. Soc. 164 (2017) F809-F814
https://doi.org/10.1149/2.0711707jes (Hybrid OA)

The large variety of resistive states in strontium titanate: Bias effects and mechanisms at high and low temperatures
M. Kubicek, S. Taibl, E. Navickas, H. Hutter, G. Fafilek, J. Fleig
J. Electroceramics 39 (2017) 197-209
https://doi.org/10.1007/s10832-017-0081-2 (Hybrid OA)

The electrochemical properties of $Sr(Ti,Fe)O_3$-d for anodes in solid oxide fuel cells
A. Nenning, L. Volgger, E. Miller, S. Barnett, J. Fleig
J. Electrochem. Soc. 164 (2017) F364-F371
https://doi.org/10.1149/2.1271704jes (Hybrid OA)

CO_2 reduction on the pre-reduced mixed ionic–electronic conducting perovskites $La_{0.6}Sr_{-0.4}FeO_{3-\delta}$ and $SrTi_{0.7}Fe_{0.3}O_{3-\delta}$ **P03/09**
M. Grenbacher, T. Götsch, A. K. Opitz, B. Klötzer, S. Penner
ChemPhysChem 19 (2018) 93-107
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Real-time impedance monitoring of oxygen reduction during surface modification of thin film cathodes
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Project Part 10 U. Schubert

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Project Part 11 J. Redinger

Adsorption of a superoxo O-2 species on the pure and Ca-doped Sr3Ru2O7(001) surface
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