

REFEREED PUBLICATIONS IN JOURNALS AND BOOKS:

Citations total number > 8000; 18 papers with more than 100 citations; h-index = 41
(source: ISI Web of Knowledge, ResearcherID: A-3681-2010, February 2012)

2012

154. Daniel Hagleitner, Peter Jacobson, Sara Blomberg, Karina Schulte, Edvin Lundgren, Markus Kubicek, Jürgen Fleig, Frank Kubel, Christoph Puls, Andreas Limbeck, Herbert Hutter, Lynn A. Boatner, Michael Schmid, Ulrike Diebold

“Bulk characterization and surface properties of $\text{In}_2\text{O}_3(100)$ single crystals”

Physical Review B, in press (February 2012)

FWF-FOXSI, ORNL

153. Ya. B. Losovyj, Shao-Chun Li, Natalia Lozova, Daniel Stellwagen, Ulrike Diebold, Lingmei Kong, Challa Kumar

“Evidence for p – d hybridization Au₃₈ gold nanoclusters”

Journal of Physical Chemistry Letters, in press (February 2012)

Center for Atomic-Level Catalyst Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number #DE-SC0001058

152. Jinke Tang, Gareth Parkinson, Ulrike Diebold, and Leszek Malkinski

“Surface and Reconstruction of Magnetic Oxides for Spintronic Applications”

Book Chapter in ‘Magnetic Materials’, Intechweb, Edited by L. Malkinski et al.,

in press (October 2011)

EFRC, LaBOR-ITRS

151. Shao-Chun Li, Peter Jacobson, Shu-Lei Zhao, Xue-Qing Gong, and Ulrike Diebold

“Trapping Nitric Oxide by Surface Hydroxyls on Rutile $\text{TiO}_2(110)$ ”

Journal of Physical Chemistry C, in press (December 2011)

dx.doi.org/10.1021/jp209290a

DE-FG02-05ER15702

150. Peter Jacobson, Bernhard Stöger, Andreas Garhofer, Gareth S. Parkinson, Michael Schmid, Roman Caudillo, Florian Mittendorfer, Josef Redinger, Ulrike Diebold

“Disorder and Defect Healing in Graphene on Ni(111)”

Journal of Physical Chemistry C Letters, 3 (2012) 136–139

dx.doi.org/10.1021/jz2015007

Intel Corp.; Austrian Science Fund (FWF) within the Wissenschaftskolleg WK04 and project I422-N16.

2011

149. G. S. Parkinson, Z. Novotny, P. Jacobson, M. Schmid, and U. Diebold

“Water Mediated Reduction of the $\text{Fe}_3\text{O}_4(001)$ Surface”

Journal of the American Chemical Society, in press (July 2011)

dx.doi.org/10.1021/ja203432e

148. S-C. Li, Y. Losovji, U. Diebold

“Adsorption-site dependent electronic structure of catechol on TiO_2 anatase (101) surface”

Langmuir 27, (2011) 8600-8604

dx.doi.org/10.1021/la201553k

147. Gareth S. Parkinson, Zbynek Novotny, Peter Jacobson, Michael Schmid, and Ulrike Diebold

“A Metastable Fe(A) Termination at the $\text{Fe}_3\text{O}_4(001)$ Surface”

Surface Science Letters, in press (March 2011)

doi:10.1016/j.susc.2011.05.018

146. Li-Min Liu, Shaochun Li, Hongzhi Cheng, Ulrike Diebold, and Annabella Selloni
“Growth and organization of an organic molecular monolayer on TiO₂: catechol on anatase (101)”
Journal of the American Chemical Society, 133 (20) (2011) 7816–7823
doi: 10.1021/ja200001r

145. Shao-Chun Li, Yaroslav Losovyi, Vinod Kumar Paliwal, and Ulrike Diebold
“Photoemission study of azobenzene and aniline adsorbed on TiO₂ anatase (101) and rutile (110) surfaces”
Journal of Physical Chemistry C 115 (20) (2011) 10173-1017
doi: 10.1021/jp202029a

144. Ulrike Diebold
“Photocatalysts: Closing the gap”, News & Views article
Nature Chemistry, 3 (2011) 271 – 272
doi:10.1038/nchem.1019

143. M. J. Uddin, D. Mondal, C. A. Morris, U. Diebold, R. D. Gonzalez
“An *in-vitro* controlled release study of valproic acid encapsulated within a titania ceramic matrix”
Applied Surface Science, 257 (2011) 7920–7927
doi:10.1016/j.apsusc.2011.03.079

2010

142. Philipp Scheiber, Alexander Riss, Michael Schmid, Peter Varga, and Ulrike Diebold
“Observation and Destruction of an Elusive Adsorbate with STM: O₂/TiO₂(110)”
Physical Review Letters, 105 (2010) 216101
Doi:10.1103/PhysRevLett.105.216101

141. Gareth Parkinson, Narasimham Mulakaluri, Yaroslav Losovji, Peter Jacobson, Rossitza Pentcheva, and Ulrike Diebold
“Adsorption-Induced Half-Metallicity at the Magnetite (001) Surface”
Physical Review B, 82 (2010) 125413
Doi: 10.1103/PhysRevB.82.125413

140. Maher Fathalla, Amelia Neuberger, Shao-Chun Li, Russell Schmehl, Ulrike Diebold, and Janarthanan Jayawickramarajah
“Straightforward Self-Assembly of Porphyrin Nanowires in Water: Harnessing Adamantane/ β -Cyclodextrin Interactions”
Journal of the American Chemical Society (Communications), 132 (2010) 9966 - 9967
Doi:10.1021/ja1030722
(Paper highlighted in Nature Materials’ Research Highlights, vol. 9, August 2010)

139. Shaochun Li, U. Diebold, Li-Na Chu, and Xue-Qing Gong
“Hydrogen controls the dynamics of catechol adsorbed on a TiO₂(110) surface”
Science 328 (2010) 882 - 884
(DE-FG02-05ER15702, CHE-0715576)
(Paper highlighted in C&EN News)

138. U. Diebold
“Oxide Surfaces: Surface Science goes Inorganic” (News & Views article)
Nature Materials, 9 (2010) 185 - 187

137. Ulrich Aschauer, Yunbin He, Hongzhi Cheng, Shao-Chun Li, Annabella Selloni, and Ulrike Diebold
“Influence of subsurface defects on the surface reactivity of TiO₂: water on anatase (101)”
Journal of Physical Chemistry C, 114 (2) (2010) 1278 - 1284
doi: 10.1021/jp910492b

136. Olga Dulub and Ulrike Diebold
“Preparation of a Pristine TiO₂ Anatase (101) Surface by Cleaving”
Journal of Physics: Condensed Matter 22 (2010) 084014
(Special Issue Honoring the Memory of Prof. T.E. Madey)
doi:10.1088/0953-8984/22/8/084014

135. (Invited Review) U. Diebold, Shao-Chun Li, and Michael Schmid
“Oxide Surface Science”
Annual Review in Physical Chemistry, 61 (2010) 131 - 148
doi: 10.1146/annurev.physchem.012809.103254
CHE-0715576, DE-FG02-05ER15702, LaBoR-ITRS, Foreign sources

134. Shao-Chun Li and Ulrike Diebold
“Reactivity of TiO₂ Rutile and Anatase Surfaces towards Nitroaromatics”
Journal of the American Chemical Society (Communication), 132 (2010) 64 – 66;
doi: 10.1021/ja907865t

2009

133. Erie H. Morales and Ulrike Diebold
“The polar ITO(001) surface: Surface structure and stabilization mechanism”
Applied Physics Letters, 95 (2009) 253105; doi:10.1063/1.3275716

132. Shao-Chun Li and Ulrike Diebold
“Direction-dependent intermolecular interactions: catechol on TiO₂(110)-1x1”
Proc. SPIE, Vol. 7396, 73960P (2009); doi:10.1117/12.828204 (July 2009)

131. Maher Fathalla, Shao-Chun Li, Ulrike Diebold, Alina Alb, Wayne Reed, and Janarthanan Jayaywickramarajah
“Water-Soluble Nanorods Self-Assembled via Pristine-C60 and Porphyrin Moieties”
Chemical Communications 28 (2009) 4209 – 42w11

130. Yunbin He, Antonio Tilocca, Olga Dulub, Annabella Selloni, and Ulrike Diebold
“Local ordering and electronic signatures of submonolayer water on anatase TiO₂(101)”
Nature Materials 8 (2009) 585 - 589

129. Yunbin He, Wei-Kun Li, Xue-Qing Gong, Olga Dulub, Annabella Selloni, and Ulrike Diebold
“Nucleation and growth of 1D water clusters on rutile TiO₂(011)-2x1”
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128. Yunbin He, Olga Dulub, Hongzhi Cheng, Annabella Selloni, and Ulrike Diebold
“Evidence for the Predominance of Subsurface Defects on TiO₂ Anatase (101)”
Physical Review Letters, 102 (10) (2009) 106105.

127. Shao-Chun Li, Jian-guo Wang, Peter Jacobson, Xueqing Gong, Annabella Selloni, and Ulrike Diebold
“Correlation between bonding geometry and band gap states at organic-inorganic interfaces: catechol on rutile TiO₂(110)”
Journal of the American Chemical Society, 131 (3) (2009) 980 - 984

126. Xue-Qing Gong, Navid Khorshidi, Andreas Stierle, Vedran Vonk, Claus Ellinger, Helmut Dosch, Hongzhi Cheng, Annabella Selloni, Yunbin He, Olga Dulub, Ulrike Diebold
“The 2×1 Reconstruction of the Rutile TiO₂(011) Surface: a Combined Density Functional Theory, X-ray Diffraction, and Scanning Tunneling Microscopy Study”
Surface Science, 603 (2009) 138 - 144

2008

125. Erie H. Morales, Yunbin He, *Ulrike Diebold*, and Bernard Delley
“Surface structure of Sn-doped In₂O₃(111) thin films by STM”
New Journal of Physics, 10 (2008) 125030
[Paper listed a ‘Best of New Journal of Physics of 2008’]

124. P. Jacobson, Shao-chun Li, Chundao Wang, and U. Diebold
“Decomposition of catechol and carbonaceous residues on TiO₂(110): A model system for cleaning of EUVL optics”
Journal of Vacuum Science and Technology B, 26 (6) (2008) 2236 - 2240

123. Shao-Chun Li, Olga Dulub and Ulrike Diebold
“Scanning Tunneling Microscopy Study of a Vicinal TiO₂ Anatase Surface”
Journal of Physical Chemistry C, 112 (2008) 16166 - 16170

122. Kh. Katsiev, A. Kolmakov, M. Fang, and U. Diebold
“Characterization of individual SnO₂ nanobelts with STM”
Surface Science Letters, 602 (2008) L112 – L114

121. Khabibullah Katsiev, Matthias Batzill, Lynn A. Boatner, and Ulrike Diebold
“Defects and Pd Growth on the Reduced SnO₂(100) Surface”
Surface Science, 602 (2008) 1699 - 1704

120. (*Invited*) *U. Diebold*
“Wiggling its way out of surface polarity: Fe₃O₄ (100) (A Perspectives on the article: A combined DFT/LEED approach for complex oxide surface structure determination: Fe₃O (011)” by R. Pentcheva, W. Moritz, J. Rundgren, S. Frank, D. Schrupp, M. Scheffler”
Surface Science, 602 (2008) 1297 - 1298

119. Xue-Qing Gong, Annabella Selloni, Olga Dulub, Peter Jacobson, and Ulrike Diebold
“Small Au and Pt clusters at the anatase TiO₂(101) surface: behavior at terraces, steps, and oxygen vacancies”
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118. P. Lascano, M. Batzill, U. Diebold, and P. Häberle
“Oxygen adsorption on Cu/ZnO (0001)-Zn”
Physical Review B 77 (2008) 035435

2007

117. M. Batzill, E. H. Morales, and U. Diebold
“Surface Studies of Nitrogen Doped TiO₂”
Chemical Physics, 339 (2007) 36 – 43

116. O. Dulub, M. Batzill, S. Solovyev, E. Loginova, A. Alchagirov, T. E. Madey, and U. Diebold
“Formation of defects on TiO₂ under electron bombardment: site-specific oxygen desorption”
Science 317 (2007) 1052 – 1056

115. (Invited) C.A. Ventrice, Jr., D.R. Borst, H. Geisler, J. van Ek, Y.B. Losovyj, P.S. Robbert, U. Diebold, J. A. Rodriguez, G.X. Miao, and A. Gupta
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Journal of Physics C: Condensed Matter, 19 (2007) 315207 - 315218 [1]
114. G. Saurav, J. Zhong, T. Siegrist, O. Dulub, U. Diebold, Y. Lu
 “Surface and Interface Properties of a-plane Mg_xZn_{1-x}O (0 ≤ x ≤ 0.3) films”
Journal of Electronic Materials, 36 (4) (2007) 446 - 451
113. K. Katsiev, M. Batzill, U. Diebold, A. Urban and B. Meyer
 “Growth of One-Dimensional Pd Nanowires on the Terraces of a Reduced SnO₂(101) Surface”
Physical Review Letters, 98 (2007) 186102
 [Article featured in the May 14, 2007 issue of Virtual Journal of Nanoscale Science & Technology] [2]
112. (Invited Review) M. Batzill and U. Diebold
 “Surface Studies of Gas Sensing Metal Oxides”
Physical Chemistry Chemical Physics, 9 (2007) 2307- 2318
 [Paper was promoted as a ‘hot article’ by PCCP]

2006

111. O. Dulub, C. Di Valentin, A. Selloni, and U. Diebold
 “Structure, Defects, and Impurities at the Rutile TiO₂(101) Surface: A Scanning Tunneling Microscopy Study
Surface Science, 600 (19) (2006) 4407- 4417
 [Paper was featured in a ‘Surface Science Perspectives’ article, written by C.L. Pang and G. Thornton entitled “The many faces of rutile titania”, Surface Science 600 (2006) 4405-4406; Paper also featured in C&EN News; Oct. 16, 2006]
110. X.-Q. Gong, A. Selloni, M. Batzill, and U. Diebold
 “Steps on TiO₂ Anatase (101)”
Nature Materials, 5 (2006) 665 -670
 [Paper featured in High Tech Materials HTM Alerts, published by the Technical Insights division of Frost & Sullivan (www.ti.frost.com)]
109. W. Wang, M. Yu, M. Batzill, J. He, U. Diebold, and J. Tang
 “Enhanced tunneling magnetoresistance and high spin polarization at room temperature in polystyrene coated Fe₃O₄ granular system through surface engineering”
Physical Review B 73 (2006) 134412
108. (Invited) M. Batzill, K. Katsiev, J.M. Burst, Y. Losvovi, W. Bergermayer, I. Tanaka, and U. Diebold
 “Tuning surface properties of SnO₂(101) by reduction”
Journal of Physics and Chemistry of Solids, 67 (9-10) (2006) 1923 – 1929
107. M. Batzill, W. Bergermayer, I. Tanaka, and U. Diebold
 “Tuning the chemical response of a gas sensitive material: Water adsorption on SnO₂(101)”
Surface Science Letters, 600 (2006) L29 – L 32
106. M. Batzill, and U. Diebold
 “Characterizing solid state gas response by surface charging in photoemission: Water adsorption on SnO₂(101)”, Journal of Physics C: Condensed Matter, 18 (2006) L129-L134.
105. M. Batzill, E.H. Morales, and U. Diebold
 “Influence of Nitrogen doping on the Surface Properties of TiO₂ Anatase and Rutile”

2005

104. M. Batzill, K. Katsiev, J.M. Burst, *U. Diebold*, A. M. Chaka, and B. Delley
"Gas-phase-dependent properties of SnO₂ (110), (100), and (101) single-crystal surfaces: Structure, composition, and electronic properties"
Physical Review B, 72 (2005) 165414
103. (Invited) O. Dulub, M. Batzill, and U. Diebold
"Growth of Copper on Single Crystalline ZnO: Surface Study of a Model Catalyst"
"Topics in Catalysis", vol. 36 (1-4) (2005) 65 – 76
102. (Invited Review) M. Batzill and U. Diebold
"The Surface and Materials Science of Tin Oxide"
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101. O. Dulub, B. Meyer, and U. Diebold
"Observation of the dynamical change in a water monolayer adsorbed on a ZnO surface"
Physical Review Letters, 95 (2005) 136101
100. C. Di Valentin, A. Tilocca, A. Selloni, T.J. Beck, A. Klust, M. Batzill, Y. Losovij, and U. Diebold
"Water adsorption on reconstructed rutile TiO₂(011)-(2x1): Ti=O double bonds and surface reactivity"
Journal of the American Chemical Society, 127, (2005) 9895-9903.
99. T.J. Beck, A. Klust, M. Batzill, U. Diebold, C. Di Valentin, A. Tilocca, and A. Selloni
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98. M. Batzill, J. M. Burst, and U. Diebold
"Pure and Co-doped SnO₂(101) Films grown by MBE on Al₂O₃"
Thin Solid Films 484 (2005) 132– 139.
97. (Invited) Ulrike Diebold
"Dispersed Au Atoms, Supported on TiO₂"
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"Optimization of synthesis variables in the preparation of active sulfated zirconia catalysts"
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95. M. Batzill, K. Katsiev, *U. Diebold*
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94. B. Meyer, D. Marx, O. Dulub, *U. Diebold*, M. Kunat, D. Langenberg, C. Wöll
"Partial Dissociation Water on the Surface of Zinc Oxide"
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93. (Invited) U. Diebold, L. Vogel Koplitz, O. Dulub

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Applied Surface Science 237 (1 - 4) (2004) 336-342

92. T.J. Beck, A. Klust, M. Batzill, U. Diebold, C. Di Valentin, A. Selloni
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"Competing Stabilization Mechanisms for the Polar ZnO(0001)-Zn Surface"
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"Dynamics of TiO₂(110) surface and step: Onset of defects in the ordered structure"
Physical Review B, 68 (2003) 233404.

88. L. Vogel Koplitz, O. Dulub, and U. Diebold
"STM study of Cu growth on ZnO(0001)-Zn and ZnO(0001bar)-O"
Journal of Physical Chemistry B, (2003) 107(38), 10583-10590.

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85. N. Ruzycski, G.S. Herman, L.A Boatner, and U. Diebold
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"Experimental Investigation on the Interaction of Water and Methanol with Anatase-TiO₂(101)"
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83. R. Marcus, U. Diebold and R. D. Gonzalez
"The Locus of Sulfate Sites on Sulfated Zirconia"
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82. (Invited) U. Diebold, "The Surface Science of Titanium Dioxide", Surface Science Reports", 48 (2003)
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(rated 'top-10 most popular articles' in ScienceDirect - Elsevier, October-November 2003, December 2003:
#3 in Materials Science, #6 in Physical and Theoretical Chemistry, #6 in Physics and Astronomy; rated 'top
1%' in the field' according to Essential Science IndicatorsT' by ISI Thomson, 2005; 'top 25 hottest articles'
in Chemistry, July-Sept 2008, ScienceDirect-Elsevier)

81. O. Dulub, U. Diebold, and G. Kresse

"Novel Stabilization Mechanism on Polar Surfaces: ZnO(0001)-Zn"
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"Variations of the Local Electronic Surface Properties of TiO₂(110) Induced by Intrinsic and Extrinsic Defects"
Physical Review B 66 (2002) 235401
- (Invited) 78. U. Diebold
"Structure and Properties of TiO₂ Surfaces: A Brief Review"
Applied Physics A 76 (2002) 1 - 7
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"STM Study of the Geometric and Electronic Structure of ZnO(0001)-Zn, (0001bar)-O, (101bar0), and (112bar0) Surfaces"
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"Understanding Metal Oxide Surfaces at the Atomic Scale: STM Investigations of Bulk-defect Dependent Surface Processes"

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