

## Publications (peer-reviewed)

Ulrike Diebold

2023

289. Oscar Gamba, Moritz Eder, Matthias Poglitsch, Panukorn Sombut, Matthias Meier, Ulrike Diebold, Michael Schmid, Gareth S. Parkinson  
“Formation and Stability of Fe-Rich Terminations of Fe<sub>3</sub>O<sub>4</sub>(001)”  
Materials Research Express, in press (November 2023)
288. Giada Franceschi, , Rene Heller, Michael Schmid, Ulrike Diebold, and Michele Riva  
“Evolution of the surface atomic structures of multielement oxide films: curse or blessing?”  
Nanoscale Advances, in press (November 2023)
287. Lena Puntischer, Panukorn Sombut, Chunlei Wang, Manuel Ulreich, Jiri Pavelec, Ali Rafsanjani-Abassi, Matthias Meier, Adam Lagin, Martin Setvin, Ulrike Diebold, Cesare Franchini, Michael Schmid and Gareth S. Parkinson  
“A Multi-Technique Study of C<sub>2</sub>H<sub>4</sub> Adsorption on Fe<sub>3</sub>O<sub>4</sub>(001)”  
Journal of Physical Chemistry C, in press (August 2023)  
[arXiv:2308.11344v1](https://arxiv.org/abs/2308.11344v1)
286. Sabrina M. Gericke, Minttu M. Kauppinen, Margareta Wagner, Michele Riva, Giada Franceschi, Alvaro Posada-Borbon, Lisa Rämisch, Sebastian Pfaff, Alexander M. Imre, Alexei B. Preobrajenski, Stephan Appelfeller, Sara Blomberg, Lindsay R. Merte, Johan Zetterberg, Ulrike Diebold, Henrik Grönbeck, and Edvin Lundgren  
“Effect of different In<sub>2</sub>O<sub>3</sub>(111) surface terminations on CO<sub>2</sub> adsorption”  
ACS Applied Materials Interfaces, in press (August 2023)  
<https://doi.org/10.1021/acsami.3c07166>  
<http://arxiv.org/abs/2308.12657>
285. Jesús Redondo, Jan Michalička, Giada Franceschi, Břetislav Šmid, Nishant Kumar, Ondrej Man, Matthias Blatnik, Dominik Wrana, Florian Kraushofer, Benjamin Mallada, Martin Švec, Gareth Parkinson, Martin Setvin, Michele Riva, Ulrike Diebold, and Jan Čechal  
„Hematite α-Fe<sub>2</sub>O<sub>3</sub>(0001) in top and side view: resolving long-standing controversies about its surface structure“  
Advanced Materials Interfaces, (July 2023) in press  
<https://doi.org/10.1002/admi.202300602>  
<https://arxiv.org/abs/2303.06023>
284. Giada Franceschi, Sebastian Brandstetter, Jan Balajka, Igor Sokolović, Jiri Pavelec, Martin Setvín, Michael Schmid, and Ulrike Diebold  
“Interaction of surface cations of cleaved mica with water in vapor and liquid forms”  
Faraday Discussions, in press, May 2023  
<https://doi.org/10.1039/D3FD00093A>  
<http://arxiv.org/abs/2308.14571>
283. Giada Franceschi and Ulrike Diebold  
“Oxide Surfaces”  
Encyclopedia of Materials: Electronic, Section: Complex Oxides, 2023, Elsevier  
[doi:10.1016/B978-0-12-819728-8.00059-0](https://doi.org/10.1016/B978-0-12-819728-8.00059-0)

282. Florian Kraushofer, Matthias Meier, Zdeněk Jakub, Johanna Hütner, Jan Balajka, Jan Hulva, Michael Schmid, Cesare Franchini, Ulrike Diebold, Gareth S. Parkinson, “Oxygen-Terminated (1×1) Reconstruction of Reduced Magnetite Fe<sub>3</sub>O<sub>4</sub>(111)” *Journal of Physical Chemistry C Letters*, 14 (2023) 3258–3265  
<https://doi.org/10.1021/acs.jpcllett.3c00281>  
[arXiv:2308.12023v1](https://arxiv.org/abs/2308.12023v1)
281. Lena Puntischer, Kevin Daninger, Michael Schmid, Ulrike Diebold, and Gareth S. Parkinson „A study of Pt, Rh, Ni and Ir dispersion on anatase TiO<sub>2</sub> (101) and the role of water” *Electrochimica Acta*, 449 (2023) 142190  
<https://doi.org/10.1016/j.electacta.2023.142190>  
<https://arxiv.org/abs/2308.11973>
280. Marco Corrias, Lorenzo Papa, Igor Sokolovic, Viktor Birschtzky, Alexander Gorfer, Martin Setvin, Michael Schmid, Ulrike Diebold, Michele Reticioli, and Cesare Franchini „Automated Real-Space Lattice Extraction for Atomic Force Microscopy Images” *Machine Learning: Science and Technology*, 4 (2023) 015015  
<https://doi.org/10.1088/2632-2153/acb5e0>  
[arXiv:2208.13286](https://arxiv.org/abs/2208.13286)
279. Giada Franceschi, Ulrike Diebold, and Jan Balajka „Atomic Structure of Oxide Surfaces in Aqueous Environment” Chapter in “Encyclopedia of Solid-Liquid Interfaces (First Edition)”, Editors: Klaus Wandelt, Gianlorenzo Bussetti Elsevier, 2024, Pages 200-209, ISBN 9780323856706  
<https://doi.org/10.1016/B978-0-323-85669-0.00078-7>
278. G. Franceschi, P. Kocán, A. Conti, S. Brandstetter, J. Balajka, I. Sokolović, M. Valtiner, F. Mittendorfer, M. Schmid, M. Setvin, and U. Diebold “Resolving the intrinsic ordering of K<sup>+</sup> ions on muscovite mica surfaces” *Nature Communications*, 14 (2023) 208  
<https://doi.org/10.1038/s41467-023-35872-y>
277. Michael Schmid, Gareth S. Parkinson and Ulrike Diebold “Analysis of temperature programmed desorption via equilibrium thermodynamics” *ACS Physical Chemistry Au*, 3 (2023) 44–62  
<https://doi.org/10.1021/acsphyschemau.2c00031>

## 2022

276. Hao Chen, Matthias Blatnik, Francesca Mirabella, Giada Franceschi, Michele Riva, Michael Schmid, Jan Čechal, Bernd Meyer, Ulrike Diebold and Margareta Wagner „Water Structures Reveal Local Hydrophobicity on the In<sub>2</sub>O<sub>3</sub>(111) Surface” *ACS Nano*, 16 (12) (2022) 21163–21173  
<https://pubs.acs.org/doi/full/10.1021/acsnano.2c09115>  
<http://arxiv.org/abs/2308.11404>
275. Zhichang Wang, Michele Reticioli, Zdenek Jakub, Igor Sokolovic, Lynn A. Boatner, Michael Schmid, Gareth S. Parkinson, Ulrike Diebold, Cesare Franchini, Martin Setvin “Surface chemistry on a polarizable surface: Coupling of CO with KTaO<sub>3</sub>(001)” *Science Advances*, 8 (2022) eabq1433,  
[DOI: 10.1126/sciadv.abq14](https://doi.org/10.1126/sciadv.abq14)

274. Michele Reticioli, Zhichang Wang, Michael Schmid, Lynn A. Boatner, Ulrike Diebold, Martin Setvin, and Cesare Franchini  
 “Competing electronic states emerging on polar surfaces”  
Nature Communications, 13 (2022) 4311  
<https://doi.org/10.1038/s41467-022-31953-6>  
[arXiv:2207.00516](https://arxiv.org/abs/2207.00516)
273. Viktor C. Birschtzky, Florian Ellinger, Michele Reticioli, Ulrike Diebold, and Cesare Franchini  
 “Machine Learning for Exploring Small Polaron Configurational Space”  
npj Computational Materials 8 (2022) 125  
<https://www.nature.com/articles/s41524-022-00805-8>  
<http://arxiv.org/abs/2202.01042>
272. Lindsay R. Merte, Malthe Kjær Bisbo, Igor Sokolovic, Martin Setvin, Benjamin Hagman, Mikhail Shipilin, Michael Schmid, Ulrike Diebold, Edwin Lundgren, and Bjørk Hammer  
 „Structure of an ultrathin tin oxide film solved by machine learning enhanced global optimization“  
Angewandte Chemie, International Edition, (2022) e202204244  
[doi: 10.1002/anie.202204244](https://doi.org/10.1002/anie.202204244)
271. Margareta Wagner, Fabio Calcinelli, Andreas Jeindl, Michael Schmid, Oliver T. Hofmann, and Ulrike Diebold,  
 “Adsorption configurations of Co-Phtalocyanine on  $\text{In}_2\text{O}_3(111)$ ”  
Surface Science, 722 (2022) 122065  
<https://doi.org/10.1016/j.susc.2022.122065>
270. Michele Reticioli, Cesare Franchini, and Ulrike Diebold  
 “Modeling polarons in density functional theory: lessons learned from  $\text{TiO}_2$ ”  
Journal of Physics Condensed Matter, 34 (2022) 204006  
<https://iopscience.iop.org/article/10.1088/1361-648X/ac58d7>
269. Matthias Meier, Jan Hulva, Zdenek Jakub, Florian Kraushofer, Mislav Bobic, Roland Bliem, Martin Setvin, Michael Schmid, Ulrike Diebold, Cesare Franchini, and Gareth S. Parkinson  
 “CO oxidation by  $\text{Pt}_2/\text{Fe}_3\text{O}_4$ : Metastable dimers and support configurations facilitate lattice oxygen extraction”  
Science Advances, 8 (2022) eabn4580  
[DOI: 10.1126/sciadv.abn4580](https://doi.org/10.1126/sciadv.abn4580)
268. Michael Schmid, David Rath and Ulrike Diebold  
 “Why and how Savitzky-Golay filters should be replaced”  
ACS Measurement Science Au, 2 (2022) 186 -196  
<https://pubs.acs.org/doi/10.1021/acsmesuresciau.1c00054>
267. Giada Franceschi, Michael Schmid, Ulrike Diebold, and Michele Riva  
 „Surface reconstructions determine surface diffusivity and the flatness of oxide surfaces“  
Journal of Vacuum Science and Technology A, 40 (2022) 023206  
<https://doi.org/10.1116/6.0001704>
266. Florian Kraushofer, Lena Haager, Moritz Eder, Ali Rafsanjani-Abbasi, Zdenek Jakub, Giada Franceschi, Michele Riva, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
 „Single Rh adatoms stabilized on  $\alpha\text{-Fe}_2\text{O}_3(1-120)$  by co-adsorbed water“  
ACS Energy Letters, 7 (2022) 375–380  
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## 2021

265. Margareta Wagner, Jakub Planer, Bettina S. J. Heller, Jens Langer, Andreas Limbeck, Lynn A. Boatner, Hans-Peter Steinrück, Josef Redinger, Florian Maier, Florian Mittendorfer, Michael Schmid and Ulrike Diebold  
“An oxygen-rich, tetrahedral surface phase on high-temperature rutile VO<sub>2</sub>(110)<sub>T</sub> single crystals”  
*Physical Review Materials*, 5 (2021) 125001  
<https://doi.org/10.1103/PhysRevMaterials.5.125001>  
<http://arxiv.org/abs/2107.00350>
264. Zdenek Jakub, Matthias Meier, Florian Kraushofer, Jan Balajka, Jiri Pavelec, Michael Schmid, Cesare Franchini, Ulrike Diebold, Gareth S. Parkinson  
“Rapid oxygen exchange at the hematite/water interface: The crucial role of surface diffusion”  
*Nature Communications*, 12 (2021) 6488  
[doi.org/10.1038/s41467-021-26601-4](https://doi.org/10.1038/s41467-021-26601-4)
263. Giada Franceschi, Michael Schmid, Rene Heller, Michael Stöger-Pollach, Ulrike Diebold, and Michele Riva  
“A 2D surface phase diagram for a multicomponent perovskite oxide: La<sub>0.8</sub>Sr<sub>0.2</sub>MnO<sub>3</sub>(110)”  
*Physical Review Materials*, 5 (2021) L092401  
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<http://arxiv.org/abs/2010.05205>
262. Francesca Mirabella, Matthias Müllner, Thomas Touzialin, Michele Riva, Zdenek Jakub, Florian Kraushofer, Michael Schmid, Marc T.M. Koper, Gareth S. Parkinson, and Ulrike Diebold  
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*Electrochimica Acta*, 389 (2021) 138639  
<https://doi.org/10.1016/j.electacta.2021.138638>
261. Igor Sokolovic, Giada Franceschi, Jian Xu, Zhichang Wang, Jiri Pavelec, Michele Riva, Michael Schmid, Ulrike Diebold, and Martin Setvin  
“The quest for a pristine, unreconstructed SrTiO<sub>3</sub>(001) surface: A study with atomically-resolved nc-AFM”  
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260. Margareta Wagner, Bernd Meyer, Martin Setvin, Michael Schmid, and Ulrike Diebold  
“Assessing of the acidity of individual surface hydroxyls”  
*Nature*, 592 (2021) 722–725  
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259. Cesare Franchini, Michele Reticcioli, Martin Setvin, and Ulrike Diebold  
“Polarons in Materials”  
*Nature Materials Reviews* (2021)  
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258. Florian Kraushofer, Nikolaus Resch, Moritz Eder, Ali Rafsanjani-Abbasi, Sarah Tobisch, Zdenek Jakub, Giada Franceschi, Michele Riva, Matthias Meier, Michael Schmid, Ulrike Diebold, Gareth S. Parkinson  
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*Advanced Materials Interfaces* (2021) 2001908  
DOI: [10.1002/admi.202001908](https://doi.org/10.1002/admi.202001908)
257. Jan Hulva, Matthias Meier, Roland Bliem, Zdenek Jakub, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson  
“Unravelling CO Adsorption on Model Single-Atom Catalysts”  
*Science*, 371 (2021) 375–379  
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256. Jakob Timmermann, Florian Kraushofer, Nikolaus Resch, Piegang Li, Yu wang, Zhiqiang Mao, Michele Riva, Yonghyuk Lee, Carsten Staacke, Michael Schmid, Christoph Scheurer, Gareth Parkinson, Ulrike Diebold, and Karsten Reuter  
“IrO<sub>2</sub> Surface Complexions Identified Through Machine Learning and Surface Investigations”  
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<https://journals.aps.org/prl/pdf/10.1103/PhysRevLett.125.206101>
255. Giada Franceschi, Michael Schmid, Ulrike Diebold, and Michele Riva  
“Atomically resolved surfaces of lanthanum-strontium manganite (110) films”  
*Journal of Materials Chemistry A*, 8 (2020) 22947–22961  
DOI: [10.1039/D0TA07032G](https://doi.org/10.1039/D0TA07032G)
254. Doris Grumelli, Tim Wiegmann, Sara Barja, Finn Reikowski, Foad Maroun, Phillipe Allongue, Jan Balajka, Gareth S. Parkinson, Ulrike Diebold, Klaus Kern, Olaf Magnussen  
“Electrochemical stability of reconstructed Fe<sub>3</sub>O<sub>4</sub>(001)”  
*Angewandte Chemie International Edition*, 59 (2020) 21904–21908  
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253. Francesca Mirabella, Jan Balajka, Jiri Pavelec, Markus Göbel, Florian Kraushofer, Michael Schmid, Gareth Parkinson and Ulrike Diebold  
“Atomic-scale studies of Fe<sub>3</sub>O<sub>4</sub>(001) and TiO<sub>2</sub>(110) surfaces following immersion in CO<sub>2</sub>-acidified water”  
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252. Martin Štubian, Juraj Bobek, Martin Setvin, Ulrike Diebold, and Michael Schmid  
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251. Giada Franceschi, Michael Schmid, Ulrike Diebold, and Michele Riva  
“Movable holder for quartz crystal microbalance for exact growth rates during pulsed laser deposition”  
*Review of Scientific Instruments*, 91 (2020) 065003  
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250. Igor Sokolović, Michele Reticcioli, Martin Calkovsyk, Margareta Wagner, Michael Schmid, , Cesare Franchini\*, Ulrike Diebold, and Martin Setvin  
“Resolving the adsorption of molecular O<sub>2</sub> on the rutile TiO<sub>2</sub>(110)-(1x1) surface by non-contact atomic force microscopy”  
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249. Giada Franceschi, Florian Kraushofer, Matthias Meier, Gareth Parkinson, Michael Schmid, Ulrike Diebold, and Michele Riva  
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*Chemistry of Materials*, in press (April 2020)  
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248. Zdenek Jakub, Jan Hulva, Paul T. P. Ryan, David A. Duncan, David J. Payne, Roland Bliem, Manuel Ulreich, Patrick Hofegger, Florian Kraushofer, Matthias Meier, Ulrike Diebold, Gareth S. Parkinson  
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247. Peter Lackner, Amy Brandt, Ulrike Diebold, and Michael Schmid  
Few-monolayer yttria-doped zirconia films: Segregation and phase stabilization  
*Journal of Chemical Physics*, 152 (2020) 064709  
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## 2019

246. Peter Lackner, Joong-Il Jake Choi, Ulrike Diebold, and Michael Schmid  
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*Journal of Materials Chemistry A*, 7 (2019) 24837–24846  
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245. Michele Riva, Giada Franceschi, Michael Schmid, and Ulrike Diebold  
“Surface Reconstructions Affect the Epitaxial Growth of Complex Oxide Thin Films”  
*Physical Review Research* 1 (September 2019) 033059  
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244. Giada Franceschi, Margareta Wagner, Jakob Hofinger, Tomáš Krajčák, Michael Schmid, Ulrike Diebold, Michele Riva  
“Growth of  $\text{In}_2\text{O}_3(111)$  Thin Films with Optimized Surfaces”  
*Physical Review Materials*, 3 (2019) 103403  
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243. Florian Kraushofer, Francesca Mirabella, Jian Xu, Jiri Pavelec, Jan Balajka, Matthias Müllner, Nikolaus Resch, Zdenek Jakub, Jan Hulva, Matthias Meier, Michael Schmid, Ulrike Diebold and Gareth Parkinson  
“Dissolution and Passivation of Magnetite: An Atomic-Scale View”  
*Journal of Chemical Physics*, 151 (2019) 154702  
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*Feature Article in J. Chem Phys Scilight "Rusting at the atomic level,"*  
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242. Peter Lackner, Zhiyu Zou, Sabrina Mayr, Ulrike Diebold, and Michael Schmid  
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241. Zdenek Jakub, Jan Hulva, Matthias Meier, Roland Bliem, Florian Kraushofer, Martin Setvin, Michael Schmid, Ulrike Diebold, Cesare Franchini, Gareth S. Parkinson  
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*Angewandte Chemie International Edition*, 7 (2019) 2559  
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240. Manuel Ulreich, Lynn A. Boatner, Igor Sokolovic, Michele Reticcioli, Berthold Stoeger, Flora Poelzleitner, Cesare Franchini, Michael Schmid, Ulrike Diebold and Martin Setvin  
“Defect chemistry of Eu dopants in NaI scintillators studied by atomically resolved force microscopy”  
*Physical Review Materials*, 3 (2019) 075004  
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239. Zdenek Jakub, Jan Hulva, Francesca Mirabella, Florian Kraushofer, Matthias Meier, Roland Bliem, Ulrike Diebold, Gareth S. Parkinson\*  
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*Journal of Physical Chemistry C*, in press (May 2019)  
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238. Michele Riva,\* Giada Franceschi, Qiyang Lu, Michael Schmid, Bilge Yildiz, Ulrike Diebold  
“Pushing the Detection of Cation Deficiency to the Limit”  
*Physical Review Materials*, **3**, 043802 (2019)  
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237. Igor Sokolovic, Michael Schmid, Ulrike Diebold, and Martin Setvin  
“Bulk-terminated SrTiO<sub>3</sub>(001): Coupling between surface defects and ferroelectricity”  
*Physical Review Materials*, **3** (2019) 034407  
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235. Michele Retliccioli, Igor Sokolovic, Michael Schmid, Ulrike Diebold, Martin Setvin, and Cesare Franchini  
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*Physical Review Letters*, **122** (2019) 016805  
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234. Peter Lackner, Zhiyu Zou, Sabrina Mayr, Joong-Il Jake Choi, Ulrike Diebold, and Michael Schmid  
“Surface structures of ZrO<sub>2</sub> films on Rh(111): From two layers to bulk termination”  
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“Adsorption of CO on the Ca<sub>3</sub>Ru<sub>2</sub>O<sub>7</sub>(001) surface”  
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## 2018

232. Matthias Müllner, Michele Riva, Florian Kraushofer, Michael Schmid, Gareth S. Parkinson, Stijn F.L. Mertens and Ulrike Diebold  
“Stability and catalytic performance of reconstructed Fe<sub>3</sub>O<sub>4</sub>(001) and Fe<sub>3</sub>O<sub>4</sub>(110) surfaces during oxygen evolution reaction”  
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231. Jan Balajka, Jiri Pavelec, Mojmir Komora, Michael Schmid, and Ulrike Diebold  
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*Review of Scientific Instruments*, **89** (2018) 083906  
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230. Peter Lackner, Jan Hulva, Eva-Maria Köck, Wernfried Mayr-Schmölzer, Joong Il J. Choi, Simon Penner, Ulrike Diebold, Florian Mittendorfer, Josef Redinger, Bernhard Klötzer, Gareth S. Parkinson, and Michael Schmid  
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"Formation and dynamics of small polarons in rutile TiO<sub>2</sub>(110) surface"  
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