Joachim Paier

List of Publications by Year
in descending order

60 papers	10,289 citations	126708 33 h-index	102304 66 g-index
68 all docs	68 docs citations	68 times ranked	11285 citing authors

#	Article	IF	Citations
1	Resolving atomic diffusion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ru</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mi mathvariant="normal">O</mml:mi><mml:mo>(</mml:mo><mml:mn>2</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>2</mml:mn><mml:mo>) with spiral high-speed scanning tunneling microscopy. Physical Review B, 2022, 105, .	1.1	4
2	Hydrogen-bond-stabilized high density catechol monolayer on magnetite Fe3O4(111). Surface Science, 2022, 719, 122027.	0.8	1
3	Formation of carbonate and oxalate species on a Cobalt-modified Fe3O4(111) surface: Comparison of DFT+U, hybrid functionals, and the random phase approximation. Surface Science, 2022, 721, 122068.	0.8	2
4	Dynamics in the O(2 Ã— 1) adlayer on Ru(0001): bridging timescales from milliseconds to minutes by scanning tunneling microscopy. Physical Chemistry Chemical Physics, 2022, 24, 15265-15270.	1.3	3
5	Electronic structure of reduced CeO2(111) surfaces interacting with hydrogen as revealed through electron energy loss spectroscopy in comparison with theoretical investigations. Journal of Electron Spectroscopy and Related Phenomena, 2021, , 147088.	0.8	6
6	Adsorption of CH4 on the Pt(111) surface: Random phase approximation compared to density functional theory. Journal of Chemical Physics, 2021, 155, 174702.	1.2	10
7	Machine Learning in Computational Surface Science and Catalysis: Case Studies on Water and Metalâ€“Oxide Interfaces. Frontiers in Chemistry, 2020, 8, 601029.	1.8	11
8	Vibrational properties of CO2 adsorbed on the Fe3O4 (111) surface: Insights gained from DFT. Journal of Chemical Physics, 2020, 152, 104702.	1.2	13
9	Elucidating Surface Structure with Action Spectroscopy. Journal of the American Chemical Society, 2020, 142, 2665-2671.	6.6	16
10	Reaction dynamics of metal/oxide catalysts: Methanol oxidation at vanadium oxide films on Rh(1Â1Â1) from UHV to 10âˆ’2 mbar. Journal of Catalysis, 2020, 385, 255-264.	3.1	13
11	Partial Oxidation of Methanol on the Fe3O4(111) Surface Studied by Density Functional Theory. Journal of Physical Chemistry C, 2019, 123, 8429-8438.	1.5	17
12	Vanadium Oxide Oligomers and Ordered Monolayers Supported on CeO₂(111): Structure and Stability Studied by Density Functional Theory. Journal of Physical Chemistry C, 2018, 122, 9101-9110.	1.5	19
13	Kooperative Bildung einer langreichweitig geordneten Wasserschicht auf der Fe₃O₄(111)â€OberflÃche. Angewandte Chemie, 2018, 130, 1423-1428.	1.6	7
14	Surface Termination of Fe₃O₄(111) Films Studied by CO Adsorption Revisited. Journal of Physical Chemistry B, 2018, 122, 527-533.	1.2	46
15	Cooperative Formation of Longâ€Range Ordering in Water Adâ€layers on Fe₃O₄(111) Surfaces. Angewandte Chemie - International Edition, 2018, 57, 1409-1413.	7.2	59
16	Water adsorption on the Fe₃O₄(111) surface: dissociation and network formation. Physical Chemistry Chemical Physics, 2018, 20, 15764-15774.	1.3	26
17	Reduction and oxidation of Au adatoms on the CeO₂(111) surface â€“ DFT+U versus hybrid functionals. Physical Chemistry Chemical Physics, 2017, 19, 12546-12558.	1.3	12
18	O₂ Activation on Ceria Catalystsâ€”The Importance of Substrate Crystallographic Orientation. Angewandte Chemie - International Edition, 2017, 56, 16399-16404.	7.2	106

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19	O₂â€Aktivierung an Cerdioxidâ€Katalysatoren â€“ Zur Bedeutung der kristallographischen Orientierung des Substrats. Angewandte Chemie, 2017, 129, 16618-16623.	1.6	21
20	Interactions of Water with the (111) and (100) Surfaces of Ceria. Journal of Physical Chemistry C, 2017, 121, 21571-21578.	1.5	33
21	Toward an Understanding of Selective Alkyne Hydrogenation on Ceria: On the Impact of O Vacancies on H₂ Interaction with CeO₂(111). Journal of the American Chemical Society, 2017, 139, 17608-17616.	6.6	120
22	Oxidative dehydrogenation of methanol at ceria-supported vanadia oligomers. Journal of Catalysis, 2017, 352, 382-387.	3.1	28
23	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. Catalysis Letters, 2016, 146, 861-885.	1.4	31
24	Structural and Electronic Effects on the Properties of Fe₂(dobdc) upon Oxidation with N₂O. Inorganic Chemistry, 2016, 55, 4924-4934.	1.9	15
25	Methanol adsorption on monocrystalline ceria surfaces. Journal of Catalysis, 2016, 336, 116-125.	3.1	34
26	Adsorption of Water on the Fe₃O₄(111) Surface: Structures, Stabilities, and Vibrational Properties Studied by Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 1056-1065.	1.5	71
27	Water Interaction with Iron Oxides. Angewandte Chemie - International Edition, 2015, 54, 13942-13946.	7.2	62
28	Surface Structure ofV2O3(0001)Revisited. Physical Review Letters, 2015, 114, 216101.	2.9	30
29	Activity versus Selectivity of the Methanol Oxidation at Ceria Surfaces: A Comparative First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 23021-23031.	1.5	31
30	Sites for Methane Activation on Lithiumâ€Doped Magnesium Oxide Surfaces. Angewandte Chemie - International Edition, 2014, 53, 8774-8778.	7.2	152
31	Catalytic Performance of Vanadium MILâ€47 and Linkerâ€Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. ChemPlusChem, 2014, 79, 1183-1197.	1.3	20
32	Support Effect in Oxide Catalysis: Methanol Oxidation on Vanadia/Ceria. Journal of the American Chemical Society, 2014, 136, 14616-14625.	6.6	101
33	Reactions of Methanol with Pristine and Defective Ceria (111) Surfaces: A Comparison of Density Functionals. Journal of Physical Chemistry C, 2014, 118, 23690-23700.	1.5	33
34	Titration of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Ce</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>+</mml:mo></mml:mrow></mml:m in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>CeO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 127 Td (stretchy="false">)</mm 2061.	2.9	55
35	Stability and migration barriers of small vanadium oxide clusters on the CeO2(111) surface studied by density functional theory. Faraday Discussions, 2013, 162, 233.	1.6	25
36	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. Chemical Reviews, 2013, 113, 3949-3985.	23.0	849

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37	Oligomeric Vanadium Oxide Species Supported on the CeO₂(111) Surface: Structure and Reactivity Studied by Density Functional Theory. Journal of Physical Chemistry C, 2013, 117, 5274-5285.	1.5	60
38	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	1.2	137
39	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	2.9	143
40	Accurate treatment of solids with the HSE screened hybrid. Physica Status Solidi (B): Basic Research, 2011, 248, 767-774.	0.7	258
41	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
42	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu a potential photovoltaic material: A hybrid Hartree-Fock density functional theory study. Physical Review B, 2009, 79, .	1.1	402
43	Second-order MÃ¸llerâ€“Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. Journal of Chemical Physics, 2009, 130, 184103.	1.2	194
44	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. Physical Review B, 2009, 80, .	1.1	47
45	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	1.1	740
46	The AM05 density functional applied to solids. Journal of Chemical Physics, 2008, 128, 084714.	1.2	220
47	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
48	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
49	Accurate band gaps and dielectric properties from one-electron theories (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064203.	0.7	1
50	Dielectric properties and excitons for extended systems from hybrid functionals. Physical Review B, 2008, 78, .	1.1	303
51	Optical spectra of Si nanocrystallites: Bethe-Salpeter approach versus time-dependent density-functional theory. Physical Review B, 2008, 78, .	1.1	64
52	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. Physical Review B, 2007, 76, .	1.1	133
53	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. Physical Review B, 2007, 75, .	1.1	288
54	Why does the B3LYP hybrid functional fail for metals?. Journal of Chemical Physics, 2007, 127, 024103.	1.2	481

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55	Screened hybrid density functionals applied to solids. Journal of Chemical Physics, 2006, 124, 154709.	1.2	1,915
56	Density functional theory study of MnO by a hybrid functional approach. Physical Review B, 2005, 72, .	1.1	160
57	The Perdewâ€“Burkeâ€“Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. Journal of Chemical Physics, 2005, 122, 234102.	1.2	754
58	Photochemistry of ethylene: A multireference configuration interaction investigation of the excited-state energy surfaces. Journal of Chemical Physics, 2004, 121, 11614-11624.	1.2	164
59	Enantioselectivity of epoxide hydrolase catalysed oxirane ring opening: a 3D QSAR study. Journal of Computer-Aided Molecular Design, 2003, 17, 1-11.	1.3	6
60	Quantitative Structureâ^'Activity Relationships for the Enantioselectivity of Oxirane Ring-Opening Catalyzed by Epoxide Hydrolases. Journal of Chemical Information and Computer Sciences, 2003, 43, 934-940.	2.8	19