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	Screened hybrid density functionals applied to solids. Journal of Chemical Physics, 2006, 124, 154709.	1.2	1,915
2	Oxygen Defects and Surface Chemistry of Ceria: Quantum Chemical Studies Compared to Experiment. Chemical Reviews, 2013, 113, 3949-3985.	23.0	849
3	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
4	Assessing the performance of recent density functionals for bulk solids. Physical Review B, 2009, 79, .	1.1	740
5	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. Physical Review B, 2008, 77, .	1.1	655
6	Hybrid functionals applied to extended systems. Journal of Physics Condensed Matter, 2008, 20, 064201.	0.7	500
7	Why does the B3LYP hybrid functional fail for metals?. Journal of Chemical Physics, 2007, 127, 024103.	1.2	481
8	<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
9	Dielectric properties and excitons for extended systems from hybrid functionals. Physical Review B, 2008, 78, .	1.1	303
10	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. Physical Review B, 2007, 75, .	1.1	288
11	Accurate treatment of solids with the HSE screened hybrid. Physica Status Solidi (B): Basic Research, 2011, 248, 767-774.	0.7	258
12	The AM05 density functional applied to solids. Journal of Chemical Physics, 2008, 128, 084714.	1.2	220
13	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
14	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
15	Density functional theory study of MnO by a hybrid functional approach. Physical Review B, 2005, 72, .	1.1	160
16	Sites for Methane Activation on Lithiumâ€Doped Magnesium Oxide Surfaces. Angewandte Chemie - International Edition, 2014, 53, 8774-8778.	7.2	152
17	van der Waals Interactions in Ionic and Semiconductor Solids. Physical Review Letters, 2011, 107, 245501.	2.9	143
18	Assessment of correlation energies based on the random-phase approximation. New Journal of Physics, 2012, 14, 043002.	1.2	137

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19	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. Physical Review B, 2007, 76, .	1.1	133
20	Hybrid functionals including random phase approximation correlation and second-order screened exchange. Journal of Chemical Physics, 2010, 132, 094103.	1.2	131
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	O₂ Activation on Ceria Catalystsâ€"The Importance of Substrate Crystallographic Orientation. Angewandte Chemie - International Edition, 2017, 56, 16399-16404.	7.2	106
23	Support Effect in Oxide Catalysis: Methanol Oxidation on Vanadia/Ceria. Journal of the American Chemical Society, 2014, 136, 14616-14625.	6.6	101
24	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
25	Optical spectra of Si nanocrystallites: Bethe-Salpeter approach versus time-dependent density-functional theory. Physical Review B, 2008, 78, .	1.1	64
26	Water Interaction with Iron Oxides. Angewandte Chemie - International Edition, 2015, 54, 13942-13946.	7.2	62
27	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
28	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
29	1 1 0 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:msup> 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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 327 Td (stretchy="false">)</mml:mo></mml:math> 2061	2.9	55
30	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. Physical Review B, 2009, 80, .	1.1	47
31	Surface Termination of Fe₃O₄(111) Films Studied by CO Adsorption Revisited. Journal of Physical Chemistry B, 2018, 122, 527-533.	1.2	46
32	Methanol adsorption on monocrystalline ceria surfaces. Journal of Catalysis, 2016, 336, 116-125.	3.1	34
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	Interactions of Water with the (111) and (100) Surfaces of Ceria. Journal of Physical Chemistry C, 2017, 121, 21571-21578.	1.5	33
35	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
36	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. Catalysis Letters, 2016, 146, 861-885.	1.4	31

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37	Surface Structure ofV2O3(0001)Revisited. Physical Review Letters, 2015, 114, 216101.	2.9	30
38	Oxidative dehydrogenation of methanol at ceria-supported vanadia oligomers. Journal of Catalysis, 2017, 352, 382-387.	3.1	28
39	Water adsorption on the Fe₃O₄(111) surface: dissociation and network formation. Physical Chemistry Chemical Physics, 2018, 20, 15764-15774.	1.3	26
40	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
41	O₂â€Aktivierung an Cerdioxidâ€Katalysatoren â€“ Zur Bedeutung der kristallographischen Orientierung des Substrats. Angewandte Chemie, 2017, 129, 16618-16623.	1.6	21
42	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
43	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
44	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
45	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
46	Elucidating Surface Structure with Action Spectroscopy. Journal of the American Chemical Society, 2020, 142, 2665-2671.	6.6	16
47	Structural and Electronic Effects on the Properties of Fe₂(dobdc) upon Oxidation with N₂O. Inorganic Chemistry, 2016, 55, 4924-4934.	1.9	15
48	Vibrational properties of CO2 adsorbed on the Fe3O4 (111) surface: Insights gained from DFT. Journal of Chemical Physics, 2020, 152, 104702.	1.2	13
49	Reaction dynamics of metal/oxide catalysts: Methanol oxidation at vanadium oxide films on Rh(1Â1Â1) from UHV to 10â"2 mbar. Journal of Catalysis, 2020, 385, 255-264.	3.1	13
50	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
51	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
52	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
53	Kooperative Bildung einer langreichweitig geordneten Wasserschicht auf der Fe₃O₄(111)â€OberflÃche. Angewandte Chemie, 2018, 130, 1423-1428.	1.6	7
54	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

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55	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
56	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:m 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:mn><mr with spiral high-speed scanning tunneling microscopy. Physical Review B, 2022, 105, .	1.1	4
57	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
58	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
59	Accurate band gaps and dielectric properties from one-electron theories (abstract only). Journal of Physics Condensed Matter, 2008, 20, 064203.	0.7	1
60	Hydrogen-bond-stabilized high density catechol monolayer on magnetite Fe3O4(111). Surface Science, 2022, 719, 122027.	0.8	1