

Joachim Paier

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

62

papers

8,562

citations

32

h-index

68

g-index

68

ext. papers

9,469

ext. citations

6.2

avg, IF

6.1

L-index

#	Paper	IF	Citations
62	Hydrogen-bond-stabilized high density catechol monolayer on magnetite Fe ₃ O ₄ (111). <i>Surface Science</i> , 2022 , 719, 122027	1.8	0
61	Formation of carbonate and oxalate species on a Cobalt-modified Fe ₃ O ₄ (111) surface: Comparison of DFT+U, hybrid functionals, and the random phase approximation. <i>Surface Science</i> , 2022 , 721, 122068	1.8	0
60	Adsorption of CH on the Pt(111) surface: Random phase approximation compared to density functional theory. <i>Journal of Chemical Physics</i> , 2021 , 155, 174702	3.9	0
59	Electronic structure of reduced CeO ₂ (111) surfaces interacting with hydrogen as revealed through electron energy loss spectroscopy in comparison with theoretical investigations. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2021 , 147088	1.7	1
58	Vibrational properties of CO adsorbed on the FeO (111) surface: Insights gained from DFT. <i>Journal of Chemical Physics</i> , 2020 , 152, 104702	3.9	6
57	Elucidating Surface Structure with Action Spectroscopy. <i>Journal of the American Chemical Society</i> , 2020 , 142, 2665-2671	16.4	9
56	Reaction dynamics of metal/oxide catalysts: Methanol oxidation at vanadium oxide films on Rh(111) from UHV to 10 ⁻² mbar. <i>Journal of Catalysis</i> , 2020 , 385, 255-264	7.3	5
55	Machine Learning in Computational Surface Science and Catalysis: Case Studies on Water and Metal-Oxide Interfaces. <i>Frontiers in Chemistry</i> , 2020 , 8, 601029	5	5
54	Partial Oxidation of Methanol on the Fe ₃ O ₄ (111) Surface Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 8429-8438	3.8	11
53	Vanadium Oxide Oligomers and Ordered Monolayers Supported on CeO ₂ (111): Structure and Stability Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 9101-9110	3.8	12
52	Kooperative Bildung einer langreichweitig geordneten Wasserschicht auf der Fe ₃ O ₄ (111)-Oberfläche. <i>Angewandte Chemie</i> , 2018 , 130, 1423-1428	3.6	2
51	Surface Termination of FeO(111) Films Studied by CO Adsorption Revisited. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 527-533	3.4	35
50	Water adsorption on the FeO(111) surface: dissociation and network formation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 15764-15774	3.6	19
49	Cooperative Formation of Long-Range Ordering in Water Ad-layers on Fe O (111) Surfaces. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 1409-1413	16.4	41
48	Reduction and oxidation of Au adatoms on the CeO(111) surface - DFT+U versus hybrid functionals. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 12546-12558	3.6	10
47	O Activation on Ceria Catalysts-The Importance of Substrate Crystallographic Orientation. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 16399-16404	16.4	74
46	O ₂ -Aktivierung an Cerdioxid-Katalysatoren Zur Bedeutung der kristallographischen Orientierung des Substrats. <i>Angewandte Chemie</i> , 2017 , 129, 16618-16623	3.6	13

45	Interactions of Water with the (111) and (100) Surfaces of Ceria. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 21571-21578	3.8	23
44	Toward an Understanding of Selective Alkyne Hydrogenation on Ceria: On the Impact of O Vacancies on H Interaction with CeO(111). <i>Journal of the American Chemical Society</i> , 2017 , 139, 17608-17616	16.4	76
43	Oxidative dehydrogenation of methanol at ceria-supported vanadia oligomers. <i>Journal of Catalysis</i> , 2017 , 352, 382-387	7.3	24
42	Methanol adsorption on monocrystalline ceria surfaces. <i>Journal of Catalysis</i> , 2016 , 336, 116-125	7.3	30
41	Adsorption of Water on the Fe ₃ O ₄ (111) Surface: Structures, Stabilities, and Vibrational Properties Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 1056-1065	3.8	56
40	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. <i>Catalysis Letters</i> , 2016 , 146, 861-885	2.8	28
39	Structural and Electronic Effects on the Properties of Fe ₂ (dobdc) upon Oxidation with N ₂ O. <i>Inorganic Chemistry</i> , 2016 , 55, 4924-34	5.1	12
38	Surface structure of V ₂ O ₃ (0001) revisited. <i>Physical Review Letters</i> , 2015 , 114, 216101	7.4	28
37	Activity versus Selectivity of the Methanol Oxidation at Ceria Surfaces: A Comparative First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 23021-23031	3.8	26
36	Water Interaction with Iron Oxides. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 13942-6	16.4	50
35	Water Interaction with Iron Oxides. <i>Angewandte Chemie</i> , 2015 , 127, 14148-14152	3.6	9
34	Catalytic Performance of Vanadium MIL-47 and Linker-Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. <i>ChemPlusChem</i> , 2014 , 79, 1183-1197	2.8	18
33	Support effect in oxide catalysis: methanol oxidation on vanadia/ceria. <i>Journal of the American Chemical Society</i> , 2014 , 136, 14616-25	16.4	82
32	Reactions of Methanol with Pristine and Defective Ceria (111) Surfaces: A Comparison of Density Functionals. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 23690-23700	3.8	31
31	Sites for methane activation on lithium-doped magnesium oxide surfaces. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 8774-8	16.4	125
30	Zentren der Methanaktivierung auf Oberflächen von Lithium-dotiertem MgO. <i>Angewandte Chemie</i> , 2014 , 126, 8919-8923	3.6	24
29	Titration of Ce ³⁺ ions in the CeO ₂ (111) surface by Au adatoms. <i>Physical Review Letters</i> , 2013 , 111, 206101	16.4	51
28	Stability and migration barriers of small vanadium oxide clusters on the CeO ₂ (111) surface studied by density functional theory. <i>Faraday Discussions</i> , 2013 , 162, 233-45	3.6	24

27	Oxygen defects and surface chemistry of ceria: quantum chemical studies compared to experiment. <i>Chemical Reviews</i> , 2013 , 113, 3949-85	68.1	675
26	Oligomeric Vanadium Oxide Species Supported on the CeO ₂ (111) Surface: Structure and Reactivity Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 5274-5285	3.8	51
25	Assessment of correlation energies based on the random-phase approximation. <i>New Journal of Physics</i> , 2012 , 14, 043002	2.9	111
24	Van der Waals interactions in ionic and semiconductor solids. <i>Physical Review Letters</i> , 2011 , 107, 245501	7.4	131
23	Accurate treatment of solids with the HSE screened hybrid. <i>Physica Status Solidi (B): Basic Research</i> , 2011 , 248, 767-774	1.3	216
22	Accurate Treatment of Solids with the HSE Screened Hybrid 2011 , 97-110		
21	Hybrid functionals including random phase approximation correlation and second-order screened exchange. <i>Journal of Chemical Physics</i> , 2010 , 132, 094103	3.9	117
20	Cu ₂ ZnSnS ₄ as a potential photovoltaic material: A hybrid Hartree-Fock density functional theory study. <i>Physical Review B</i> , 2009 , 79,	3.3	372
19	Second-order Møller-Plesset perturbation theory applied to extended systems. I. Within the projector-augmented-wave formalism using a plane wave basis set. <i>Journal of Chemical Physics</i> , 2009 , 130, 184103	3.9	167
18	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. <i>Physical Review B</i> , 2009 , 80,	3.3	42
17	Assessing the performance of recent density functionals for bulk solids. <i>Physical Review B</i> , 2009 , 79,	3.3	530
16	The AM05 density functional applied to solids. <i>Journal of Chemical Physics</i> , 2008 , 128, 084714	3.9	196
15	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. <i>Physical Review B</i> , 2008 , 77,	3.3	613
14	Hybrid functionals applied to extended systems. <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 064201	1.8	430
13	Accurate band gaps and dielectric properties from one-electron theories (abstract only). <i>Journal of Physics Condensed Matter</i> , 2008 , 20, 064203	1.8	1
12	Dielectric properties and excitons for extended systems from hybrid functionals. <i>Physical Review B</i> , 2008 , 78,	3.3	267
11	Optical spectra of Si nanocrystallites: Bethe-Salpeter approach versus time-dependent density-functional theory. <i>Physical Review B</i> , 2008 , 78,	3.3	61
10	Why does the B3LYP hybrid functional fail for metals?. <i>Journal of Chemical Physics</i> , 2007 , 127, 024103	3.9	424

9	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. <i>Physical Review B</i> , 2007 , 76,	3.3	121
8	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. <i>Physical Review B</i> , 2007 , 75,	3.3	259
7	Screened hybrid density functionals applied to solids. <i>Journal of Chemical Physics</i> , 2006 , 124, 154709	3.9	1591
6	Density functional theory study of MnO by a hybrid functional approach. <i>Physical Review B</i> , 2005 , 72,	3.3	147
5	The Perdew-Burke-Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. <i>Journal of Chemical Physics</i> , 2005 , 122, 234102	3.9	560
4	Photochemistry of ethylene: a multireference configuration interaction investigation of the excited-state energy surfaces. <i>Journal of Chemical Physics</i> , 2004 , 121, 11614-24	3.9	150
3	Enantioselectivity of epoxide hydrolase catalysed oxirane ring opening: a 3D QSAR study. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 1-11	4.2	5
2	Quantitative structure-activity relationships for the enantioselectivity of oxirane ring-opening catalyzed by epoxide hydrolases. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 934-40		16
1	Dynamics in the O(2 $\sqrt{3}$) adlayer on Ru(0001): bridging timescales from milliseconds to minutes by scanning tunneling microscopy. <i>Physical Chemistry Chemical Physics</i> ,	3.6	1