Joachim Paier

List of Publications by Citations

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	Screened hybrid density functionals applied to solids. *Journal of Chemical Physics*, **2006**, 124, 154709	3.9	1591
61	Oxygen defects and surface chemistry of ceria: quantum chemical studies compared to experiment. *Chemical Reviews*, **2013**, 113, 3949-85	68.1	675
60	Defect energetics in ZnO: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2008**, 77,	3.3	613
59	The Perdew-Burke-Ernzerhof exchange-correlation functional applied to the G2-1 test set using a plane-wave basis set. *Journal of Chemical Physics*, **2005**, 122, 234102	3.9	560
58	Assessing the performance of recent density functionals for bulk solids. *Physical Review B*, **2009**, 79,	3.3	530
57	Hybrid functionals applied to extended systems. *Journal of Physics Condensed Matter*, **2008**, 20, 064201	1.8	430
56	Why does the B3LYP hybrid functional fail for metals?. *Journal of Chemical Physics*, **2007**, 127, 024103	3.9	424
55	Cu2ZnSnS4 as a potential photovoltaic material: A hybrid Hartree-Fock density functional theory study. *Physical Review B*, **2009**, 79,	3.3	372
54	Dielectric properties and excitons for extended systems from hybrid functionals. *Physical Review B*, **2008**, 78,	3.3	267
53	Ground-state properties of multivalent manganese oxides: Density functional and hybrid density functional calculations. *Physical Review B*, **2007**, 75,	3.3	259
52	Accurate treatment of solids with the HSE screened hybrid. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 767-774	1.3	216
51	The AM05 density functional applied to solids. *Journal of Chemical Physics*, **2008**, 128, 084714	3.9	196
50	Second-order Møller-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	3.9	167
49	Photochemistry of ethylene: a multireference configuration interaction investigation of the excited-state energy surfaces. *Journal of Chemical Physics*, **2004**, 121, 11614-24	3.9	150
48	Density functional theory study of MnO by a hybrid functional approach. *Physical Review B*, **2005**, 72,	3.3	147
47	Van der Waals interactions in ionic and semiconductor solids. *Physical Review Letters*, **2011**, 107, 245501	7.4	131
46	Sites for methane activation on lithium-doped magnesium oxide surfaces. *Angewandte Chemie - International Edition*, **2014**, 53, 8774-8	16.4	125

45	CO adsorption on metal surfaces: A hybrid functional study with plane-wave basis set. *Physical Review B*, **2007**, 76,	3.3	121
44	Hybrid functionals including random phase approximation correlation and second-order screened exchange. *Journal of Chemical Physics*, **2010**, 132, 094103	3.9	117
43	Assessment of correlation energies based on the random-phase approximation. *New Journal of Physics*, **2012**, 14, 043002	2.9	111
42	Support effect in oxide catalysis: methanol oxidation on vanadia/ceria. *Journal of the American Chemical Society*, **2014**, 136, 14616-25	16.4	82
41	Toward an Understanding of Selective Alkyne Hydrogenation on Ceria: On the Impact of O Vacancies on H Interaction with CeO(111). *Journal of the American Chemical Society*, **2017**, 139, 17608-17618	16.4	76
40	O Activation on Ceria Catalysts-The Importance of Substrate Crystallographic Orientation. *Angewandte Chemie - International Edition*, **2017**, 56, 16399-16404	16.4	74
39	Optical spectra of Si nanocrystallites: Bethe-Salpeter approach versus time-dependent density-functional theory. *Physical Review B*, **2008**, 78,	3.3	61
38	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	3.8	56
37	Titration of Ce3+ ions in the CeO2(111) surface by Au adatoms. *Physical Review Letters*, **2013**, 111, 206101	7.4	51
36	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	3.8	51
35	Water Interaction with Iron Oxides. *Angewandte Chemie - International Edition*, **2015**, 54, 13942-6	16.4	50
34	Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. *Physical Review B*, **2009**, 80,	3.3	42
33	Cooperative Formation of Long-Range Ordering in Water Ad-layers on Fe O (111) Surfaces. *Angewandte Chemie - International Edition*, **2018**, 57, 1409-1413	16.4	41
32	Surface Termination of FeO(111) Films Studied by CO Adsorption Revisited. *Journal of Physical Chemistry B*, **2018**, 122, 527-533	3.4	35
31	Reactions of Methanol with Pristine and Defective Ceria (111) Surfaces: A Comparison of Density Functionals. *Journal of Physical Chemistry C*, **2014**, 118, 23690-23700	3.8	31
30	Methanol adsorption on monocrystalline ceria surfaces. *Journal of Catalysis*, **2016**, 336, 116-125	7.3	30
29	Surface structure of V_{2}O_{3}(0001) revisited. *Physical Review Letters*, **2015**, 114, 216101	7.4	28
28	Hybrid Density Functionals Applied to Complex Solid Catalysts: Successes, Limitations, and Prospects. *Catalysis Letters*, **2016**, 146, 861-885	2.8	28

27	Activity versus Selectivity of the Methanol Oxidation at Ceria Surfaces: A Comparative First-Principles Study. *Journal of Physical Chemistry C*, **2015**, 119, 23021-23031	3.8	26
26	Stability and migration barriers of small vanadium oxide clusters on the CeO2(111) surface studied by density functional theory. *Faraday Discussions*, **2013**, 162, 233-45	3.6	24
25	Oxidative dehydrogenation of methanol at ceria-supported vanadia oligomers. *Journal of Catalysis*, **2017**, 352, 382-387	7.3	24
24	Zentren der Methanaktivierung auf Oberflächen von Lithium-dotiertem MgO. *Angewandte Chemie*, **2014**, 126, 8919-8923	3.6	24
23	Interactions of Water with the (111) and (100) Surfaces of Ceria. *Journal of Physical Chemistry C*, **2017**, 121, 21571-21578	3.8	23
22	Water adsorption on the FeO(111) surface: dissociation and network formation. *Physical Chemistry Chemical Physics*, **2018**, 20, 15764-15774	3.6	19
21	Catalytic Performance of Vanadium MIL-47 and Linker-Substituted Variants in the Oxidation of Cyclohexene: A Combined Theoretical and Experimental Approach. *ChemPlusChem*, **2014**, 79, 1183-1197	2.8	18
20	Quantitative structure-activity relationships for the enantioselectivity of oxirane ring-opening catalyzed by epoxide hydrolases. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 934-40		16
19	O2-Aktivierung an Cerdioxid-Katalysatoren Zur Bedeutung der kristallographischen Orientierung des Substrats. *Angewandte Chemie*, **2017**, 129, 16618-16623	3.6	13
18	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	3.8	12
17	Structural and Electronic Effects on the Properties of Fe2(dobdc) upon Oxidation with N2O. *Inorganic Chemistry*, **2016**, 55, 4924-34	5.1	12
16	Partial Oxidation of Methanol on the Fe3O4(111) Surface Studied by Density Functional Theory. *Journal of Physical Chemistry C*, **2019**, 123, 8429-8438	3.8	11
15	Reduction and oxidation of Au adatoms on the CeO(111) surface - DFT+U versus hybrid functionals. *Physical Chemistry Chemical Physics*, **2017**, 19, 12546-12558	3.6	10
14	Elucidating Surface Structure with Action Spectroscopy. *Journal of the American Chemical Society*, **2020**, 142, 2665-2671	16.4	9
13	Water Interaction with Iron Oxides. *Angewandte Chemie*, **2015**, 127, 14148-14152	3.6	9
12	Vibrational properties of CO adsorbed on the FeO (111) surface: Insights gained from DFT. *Journal of Chemical Physics*, **2020**, 152, 104702	3.9	6
11	Reaction dynamics of metal/oxide catalysts: Methanol oxidation at vanadium oxide films on Rh(1□1□1) from UHV to 10□ mbar. *Journal of Catalysis*, **2020**, 385, 255-264	7.3	5
10	Enantioselectivity of epoxide hydrolase catalysed oxirane ring opening: a 3D QSAR study. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 1-11	4.2	5

9	Machine Learning in Computational Surface Science and Catalysis: Case Studies on Water and Metal-Oxide Interfaces. *Frontiers in Chemistry*, **2020**, 8, 601029	5	5
8	Kooperative Bildung einer langreichweitig geordneten Wasserschicht auf der Fe3O4(111)-Oberfl□he. *Angewandte Chemie*, **2018**, 130, 1423-1428	3.6	2
7	Accurate band gaps and dielectric properties from one-electron theories (abstract only). *Journal of Physics Condensed Matter*, **2008**, 20, 064203	1.8	1
6	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	1.7	1
5	Dynamics in the O(2 □1) adlayer on Ru(0001): bridging timescales from milliseconds to minutes by scanning tunneling microscopy. *Physical Chemistry Chemical Physics*,	3.6	1
4	Hydrogen-bond-stabilized high density catechol monolayer on magnetite Fe3O4(111). *Surface Science*, **2022**, 719, 122027	1.8	0
3	Adsorption of CH on the Pt(111) surface: Random phase approximation compared to density functional theory. *Journal of Chemical Physics*, **2021**, 155, 174702	3.9	0
2	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	1.8	0
1	Accurate Treatment of Solids with the HSE Screened Hybrid **2011**, 97-110		