Bernd Meyer

List of Publications by Year
in descending order

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71 papers	3,678 citations	172207 29 h-index	128067 60 g-index
74 all docs	74 docs citations	74 times ranked	5307 citing authors

#	Article	IF	Citations
1	Density-functional study of the structure and stability of ZnO surfaces. Physical Review B, 2003, 67, .	1.1	536
2	Partial Dissociation of Water Leads to Stable Superstructures on the Surface of Zinc Oxide. Angewandte Chemie - International Edition, 2004, 43, 6641-6645.	7.2	253
3	First-principles study of the polar O-terminated ZnO surface in thermodynamic equilibrium with oxygen and hydrogen. Physical Review B, 2004, 69, .	1.1	245
4	Composition, structure, and stability of the rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Oxygen depletion, hydroxylation, hydrogen migration, and water adsorption. Physical Review B, 2009, 79, .	1.1	226
5	Active Sites on Oxide Surfaces: ZnO-Catalyzed Synthesis of Methanol from CO and H2. Angewandte Chemie - International Edition, 2005, 44, 2790-2794.	7.2	192
6	Dislocations in bilayer graphene. Nature, 2014, 505, 533-537.	13.7	185
7	Observation of the Dynamical Change in a Water Monolayer Adsorbed on a ZnO Surface. Physical Review Letters, 2005, 95, 136101.	2.9	176
8	Water adsorption on ZnO(101Ì„0): from single molecules to partially dissociated monolayers. Physical Chemistry Chemical Physics, 2006, 8, 1513.	1.3	150
9	Concaveâ€“Convex Ï€â€“Ï€ Template Approach Enables the Synthesis of [10]Cycloparaphenyleneâ€“Fullerene [2]Rotaxanes. Journal of the American Chemical Society, 2018, 140, 13413-13420.	6.6	119
10	Phosphonate- and Carboxylate-Based Self-Assembled Monolayers for Organic Devices: A Theoretical Study of Surface Binding on Aluminum Oxide with Experimental Support. ACS Applied Materials & Interfaces, 2013, 5, 6073-6080.	4.0	111
11	CO2 Activation by ZnO through the Formation of an Unusual Tridentate Surface Carbonate. Angewandte Chemie - International Edition, 2007, 46, 5624-5627.	7.2	98
12	Density-functional study ofCuatoms, monolayers, films, and coadsorbates on polarZnOsurfaces. Physical Review B, 2004, 69, .	1.1	85
13	Effect of friction on oxidative graphite intercalation and high-quality graphene formation. Nature Communications, 2018, 9, 836.	5.8	79
14	Experimental and Theoretical Assessment of Niâ€Based Binary Compounds for the Hydrogen Evolution Reaction. Advanced Energy Materials, 2017, 7, 1601735.	10.2	77
15	Schottky barriers at transition-metal/<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2009, 79, .	1.1	75
16	Highly Strained, Radially Ï€-Conjugated Porphyrinylene Nanohoops. Journal of the American Chemical Society, 2019, 141, 18500-18507.	6.6	64
17	Ecov- a new tool for the analysis of electronic structure data in a chemical language. Journal of Physics Condensed Matter, 1999, 11, L287-L293.	0.7	57
18	Fâ€…Centers versus Dimer Vacancies on ZnO Surfaces: Characterization by STM and STS Calculations. Angewandte Chemie - International Edition, 2007, 46, 4894-4897.	7.2	46

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19	Composite Nanostructures of TiO₂ and ZnO for Water Splitting Application: Atomic Layer Deposition Growth and Density Functional Theory Investigation. Advanced Functional Materials, 2016, 26, 4882-4889.	7.8	44
20	Methanol synthesis on ZnO(0001Â¯). I. Hydrogen coverage, charge state of oxygen vacancies, and chemical reactivity. Journal of Chemical Physics, 2009, 130, 184706.	1.2	43
21	Direct assessment of the acidity of individual surface hydroxyls. Nature, 2021, 592, 722-725.	13.7	43
22	â€œInvertedâ€•porphyrins: a distorted adsorption geometry of free-base porphyrins on Cu(111). Chemical Communications, 2017, 53, 8207-8210.	2.2	38
23	Resolving the Structure of a Well-Ordered Hydroxyl Overlayer on In₂O₃(111): Nanomanipulation and Theory. ACS Nano, 2017, 11, 11531-11541.	7.3	37
24	Porphyrin Metalation at MgO Surfaces: A Spectroscopic and Quantum Mechanical Study on Complementary Model Systems. Chemistry - A European Journal, 2016, 22, 1744-1749.	1.7	36
25	Ab initiocalculations of ferroelectric instability in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>PbTiO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>with symmetric and asymmetric electrode layers. Physical Review B, 2009, 80, .	1.1	35
26	Dynamic Covalent Formation of Concave Disulfide Macrocycles Mechanically Interlocked with Singleâ€Walled Carbon Nanotubes. Angewandte Chemie - International Edition, 2020, 59, 18774-18785.	7.2	35
27	Firstâ€principles study of the reconstruction and hydroxylation of the polar NiO(111) surface. Physica Status Solidi (B): Basic Research, 2011, 248, 2229-2241.	0.7	34
28	Parameterization of tight-binding models from density functional theory calculations. Physical Review B, 2011, 84, .	1.1	33
29	Tuning the Reactivity of a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Cu</mml:mi><mml:mo>/</mml:mo><mml:mi>ZnO</mml:mi></mml:math>Nanocatalyst via Gas Phase Pressure. Physical Review Letters, 2013, 110, 086108.	2.9	31
30	Adsorption Behavior of a Cyano-Functionalized Porphyrin on Cu(111) and Ag(111): From Molecular Wires to Ordered Supramolecular Two-Dimensional Aggregates. Journal of Physical Chemistry C, 2017, 121, 26361-26371.	1.5	29
31	Reducing the In₂O₃(111) Surface Results in Ordered Indium Adatoms. Advanced Materials Interfaces, 2014, 1, 1400289.	1.9	26
32	Substrate-Modulated Reductive Graphene Functionalization. Angewandte Chemie - International Edition, 2016, 55, 14858-14862.	7.2	26
33	Perfect and Controllable Nesting in Minimally Twisted Bilayer Graphene. Nano Letters, 2020, 20, 971-978.	4.5	26
34	Chemisorption and Physisorption at the Metal/Organic Interface: Bond Energies of Naphthalene and Azulene on Coinage Metal Surfaces. Journal of Physical Chemistry C, 2020, 124, 8257-8268.	1.5	26
35	Controlling the Selfâ€Metalation Rate of Tetraphenylporphyrins on Cu(111) via Cyano Functionalization. Angewandte Chemie - International Edition, 2018, 57, 10074-10079.	7.2	24
36	Development of orthogonal tight-binding models for Ti-C and Ti-N systems. Physical Review B, 2011, 84, .	1.1	23

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37	Adsorbate-induced lifting of substrate relaxation is a general mechanism governing titania surface chemistry. Nature Communications, 2016, 7, 12888.	5.8	23
38	Enhanced sampling and free energy calculations with hybrid functionals and plane waves for chemical reactions. Journal of Chemical Physics, 2018, 149, 144113.	1.2	22
39	Microstructure, Mechanical Properties and Tribological Behavior of Magnetron-Sputtered MoS2 Solid Lubricant Coatings Deposited under Industrial Conditions. Coatings, 2021, 11, 455.	1.2	21
40	Ab initio analysis of electron energy loss spectra for complex oxides. Ultramicroscopy, 1999, 80, 145-151.	0.8	20
41	Moleculeâ€“Metal Bond of Alternant versus Nonalternant Aromatic Systems on Coinage Metal Surfaces: Naphthalene versus Azulene on Ag(111) and Cu(111). Journal of Physical Chemistry C, 2019, 123, 29219-29230.	1.5	20
42	Methanol synthesis on ZnO($mathrm{m{{000overline{1}}}}$0001Ì„). II. Structure, energetics, and vibrational signature of reaction intermediates. Journal of Chemical Physics, 2013, 139, 044705.	1.2	16
43	Methanol synthesis on ZnO from molecular dynamics. Physica Status Solidi (B): Basic Research, 2013, 250, 1174-1190.	0.7	16
44	Interface Chemistry and Molecular Bonding of Functional Ethoxysilane-Based Self-Assembled Monolayers on Magnesium Surfaces. ACS Applied Materials & Interfaces, 2015, 7, 9006-9014.	4.0	16
45	Self-Assembly and Stability of Hydrogen-Bonded Networks of Bridged Triphenylamines on Au(111) and Cu(111). Journal of Physical Chemistry C, 2015, 119, 25945-25955.	1.5	13
46	Formation of Highly Ordered Molecular Porous 2D Networks from Cyanoâ€Functionalized Porphyrins on Cu(111). Chemistry - A European Journal, 2020, 26, 13408-13418.	1.7	12
47	Etching of Crystalline ZnO Surfaces upon Phosphonic Acid Adsorption: Guidelines for the Realization of Well-Engineered Functional Self-Assembled Monolayers. ACS Applied Materials & Interfaces, 2016, 8, 13472-13483.	4.0	11
48	Formation and Stability of Phenylphosphonic Acid Monolayers on ZnO: Comparison of In Situ and Ex Situ SAM Preparation. Langmuir, 2016, 32, 5029-5037.	1.6	11
49	Bicanonical ab Initio Molecular Dynamics for Open Systems. Journal of Chemical Theory and Computation, 2017, 13, 3455-3469.	2.3	10
50	Cubic C₈: An Observable Allotrope of Carbon?. ChemPhysChem, 2015, 16, 2165-2171.	1.0	9
51	Well-Ordered In Adatoms at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>In</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:mo>−</mml:mo><mml:msub><mml:mrow><mml:mi mathvariant="normal">O</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 172 Td (stretchy="false">)</mml:mo></mml:mrow></mml:math> Surface. Physical Review Letters, 2016, 117, 206101.	9	9
52	Structural reorientation and compaction of porous MoS2 coatings during wear testing. Wear, 2022, 500-501, 204339.	1.5	9
53	Influence of Tail Groups during Functionalization of ZnO Nanoparticles on Binding Enthalpies and Photoluminescence. Langmuir, 2017, 33, 13581-13589.	1.6	8
54	Kontrolle der Selbstmetallierungsrate von Tetraphenylporphyrinen auf Cu(111) durch Funktionalisierung mit Cyangruppen. Angewandte Chemie, 2018, 130, 10230-10236.	1.6	8

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55	Mechanische Verzahnung von einwandigen Kohlenstoffnanorähren durch dynamischâ€kovalente Bildung von konkaven Disulfidmakrozyklen. Angewandte Chemie, 2020, 132, 18933-18945.	1.6	8
56	Integrating state of the art compute, communication, and autotuning strategies to multiply the performance of ab initio molecular dynamics on massively parallel multi-core supercomputers. Computer Physics Communications, 2021, 260, 107745.	3.0	8
57	Binary supramolecular networks of bridged triphenylamines with different substituents and identical scaffolds. Chemical Communications, 2018, 54, 11554-11557.	2.2	7
58	Adsorption energies of porphyrins on MgO(100): An experimental benchmark for dispersion-corrected density-functional theory. Surface Science, 2022, 717, 121979.	0.8	7
59	Adsorption of sulfur mustard on clean and water-saturated ZnO(10<mml:math) 1j ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 597 Td (x calculations. Journal of Hazardous Materials, 2021, 402, 123503.	6.5	5
60	Tunable Photoswitching in Norbornadiene (NBD)/Quadricyclane (QC) â€“ Fullerene Hybrids. Chemistry - A European Journal, 2021, 27, 14501-14507.	1.7	5
61	Improving the scaling and performance of multiple time steppingâ€based molecular dynamics with hybrid density functionals. Journal of Computational Chemistry, 2022, , .	1.5	5
62	Frequencies and polarization vectors of phonons: Results from force constants which are fitted to experimental data or calculatedab initio. Physical Review B, 2012, 86, .	1.1	4
63	Impact of twin boundaries on bulk elastic constants: Density-functional theory data for Young×³s modulus of Ag. Data in Brief, 2015, 3, 209-215.	0.5	4
64	Single-walled carbon nanotubes in tetrahydrofuran solution: microsolvation from first-principles calculations. Journal of Molecular Modeling, 2019, 25, 206.	0.8	3
65	Atomically resolved TEM imaging of covalently functionalised graphene. Npj 2D Materials and Applications, 2022, 6, .	3.9	3
66	Adsorption and self-assembly of a mono-cyano Zn-tetraphenylporphyrin derivative on KBr(001) and MgO(001). Surface Science, 2022, , 122097.	0.8	1
67	Resolution of Intramolecular Dipoles and a Push-Back Effect of Individual Molecules on a Metal Surface. Journal of Physical Chemistry C, 2022, 126, 7667-7673.	1.5	1
68	Hidden Defects and Unexpected Properties of Graphene â€” How Advanced TEM Contributes to Materials Development. Microscopy and Microanalysis, 2017, 23, 1752-1753.	0.2	0
69	Frontispiz: Kontrolle der Selbstmetallierungsrate von Tetraphenylporphyrinen auf Cu(111) durch Funktionalisierung mit Cyangruppen. Angewandte Chemie, 2018, 130, .	1.6	0
70	Frontispiece: Controlling the Self-Metalation Rate of Tetraphenylporphyrins on Cu(111) via Cyano Functionalization. Angewandte Chemie - International Edition, 2018, 57, .	7.2	0
71	General relation between stacking order and Chern index: A topological map of minimally twisted bilayer graphene. Physical Review B, 2021, 104, .	1.1	0