Bernd Meyer

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4062631/publications.pdf

Version: 2024-02-01

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	Adsorption energies of porphyrins on MgO(100): An experimental benchmark for dispersion-corrected density-functional theory. Surface Science, 2022, 717, 121979.	0.8	7
2	Improving the scaling and performance of multiple time steppingâ€based molecular dynamics with hybrid density functionals. Journal of Computational Chemistry, 2022, , .	1.5	5
3	Structural reorientation and compaction of porous MoS2 coatings during wear testing. Wear, 2022, 500-501, 204339.	1.5	9
4	Adsorption and self-assembly of a mono-cyano Zn-tetraphenylporphyrin derivative on KBr(001) and MgO(001). Surface Science, 2022, , 122097.	0.8	1
5	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
6	Atomically resolved TEM imaging of covalently functionalised graphene. Npj 2D Materials and Applications, 2022, 6, .	3.9	3
7	Adsorption of sulfur mustard on clean and water-saturated ZnO(10<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 517 Td (x calculations. Journal of Hazardous Materials, 2021, 402, 123503.	6.5	5
8	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
9	Direct assessment of the acidity of individual surface hydroxyls. Nature, 2021, 592, 722-725.	13.7	43
10	Microstructure, Mechanical Properties and Tribological Behavior of Magnetron-Sputtered MoS2 Solid Lubricant Coatings Deposited under Industrial Conditions. Coatings, 2021, 11, 455.	1.2	21
11	General relation between stacking order and Chern index: A topological map of minimally twisted bilayer graphene. Physical Review B, 2021, 104, .	1.1	0
12	Tunable Photoswitching in Norbornadiene (NBD)/Quadricyclane (QC) â€“ Fullerene Hybrids. Chemistry - A European Journal, 2021, 27, 14501-14507.	1.7	5
13	Perfect and Controllable Nesting in Minimally Twisted Bilayer Graphene. Nano Letters, 2020, 20, 971-978.	4.5	26
14	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
15	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
16	Mechanische Verzahnung von einwandigen KohlenstoffnanorÃ¶hren durch dynamischâ€kovalente Bildung von konkaven Disulfidmakrozyklen. Angewandte Chemie, 2020, 132, 18933-18945.	1.6	8
17	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
18	Single-walled carbon nanotubes in tetrahydrofuran solution: microsolvation from first-principles calculations. Journal of Molecular Modeling, 2019, 25, 206.	0.8	3

#	Article	IF	Citations
19	Highly Strained, Radially Ï€-Conjugated Porphyrinylene Nanohoops. Journal of the American Chemical Society, 2019, 141, 18500-18507.	6.6	64
20	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
21	Effect of friction on oxidative graphite intercalation and high-quality graphene formation. Nature Communications, 2018, 9, 836.	5.8	79
22	Kontrolle der Selbstmetallierungsrate von Tetraphenylporphyrinen auf Cu(111) durch Funktionalisierung mit Cyangruppen. Angewandte Chemie, 2018, 130, 10230-10236.	1.6	8
23	Controlling the Selfâ€Metalation Rate of Tetraphenylporphyrins on Cu(111) via Cyano Functionalization. Angewandte Chemie - International Edition, 2018, 57, 10074-10079.	7.2	24
24	Frontispiz: Kontrolle der Selbstmetallierungsrate von Tetraphenylporphyrinen auf Cu(111) durch Funktionalisierung mit Cyangruppen. Angewandte Chemie, 2018, 130, .	1.6	0
25	Frontispiece: Controlling the Self-Metalation Rate of Tetraphenylporphyrins on Cu(111) via Cyano Functionalization. Angewandte Chemie - International Edition, 2018, 57, .	7.2	0
26	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
27	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
28	Binary supramolecular networks of bridged triphenylamines with different substituents and identical scaffolds. Chemical Communications, 2018, 54, 11554-11557.	2.2	7
29	Resolving the Structure of a Well-Ordered Hydroxyl Overlayer on In₂O₃(111): Nanomanipulation and Theory. ACS Nano, 2017, 11, 11531-11541.	7.3	37
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	â€œInvertedâ€•porphyrins: a distorted adsorption geometry of free-base porphyrins on Cu(111). Chemical Communications, 2017, 53, 8207-8210.	2.2	38
32	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
33	Influence of Tail Groups during Functionalization of ZnO Nanoparticles on Binding Enthalpies and Photoluminescence. Langmuir, 2017, 33, 13581-13589.	1.6	8
34	Bicanonical ab Initio Molecular Dynamics for Open Systems. Journal of Chemical Theory and Computation, 2017, 13, 3455-3469.	2.3	10
35	Experimental and Theoretical Assessment of Niâ€Based Binary Compounds for the Hydrogen Evolution Reaction. Advanced Energy Materials, 2017, 7, 1601735.	10.2	77
36	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

#	Article	IF	Citations
37	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
38	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
39	Adsorbate-induced lifting of substrate relaxation is a general mechanism governing titania surface chemistry. Nature Communications, 2016, 7, 12888.	5.8	23
40	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:mrow><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:mrow><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 612 Td (stretchy="false">)</mml:mo></mml:mrow></mml:math> Surface. Physical Review Letters, 2016, 117, 206101.	2.9	9
41	Substrate-Modulated Reductive Graphene Functionalization. Angewandte Chemie - International Edition, 2016, 55, 14858-14862.	7.2	26
42	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
43	Cubic C₈: An Observable Allotrope of Carbon?. ChemPhysChem, 2015, 16, 2165-2171.	1.0	9
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	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
46	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
47	Dislocations in bilayer graphene. Nature, 2014, 505, 533-537.	13.7	185
48	Reducing the In₂O₃(111) Surface Results in Ordered Indium Adatoms. Advanced Materials Interfaces, 2014, 1, 1400289.	1.9	26
49	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
50	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
51	Methanol synthesis on ZnO from molecular dynamics. Physica Status Solidi (B): Basic Research, 2013, 250, 1174-1190.	0.7	16
52	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
53	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
54	Parameterization of tight-binding models from density functional theory calculations. Physical Review B, 2011, 84, .	1.1	33

#	Article	IF	Citations
55	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
56	Development of orthogonal tight-binding models for Ti-C and Ti-N systems. Physical Review B, 2011, 84, .	1.1	23
57	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
58	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	76
59	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
60	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
61	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
62	CO2 Activation by ZnO through the Formation of an Unusual Tridentate Surface Carbonate. Angewandte Chemie - International Edition, 2007, 46, 5624-5627.	7.2	98
63	Water adsorption on ZnO(101Ì„0): from single molecules to partially dissociated monolayers. Physical Chemistry Chemical Physics, 2006, 8, 1513.	1.3	150
64	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
65	Observation of the Dynamical Change in a Water Monolayer Adsorbed on a ZnO Surface. Physical Review Letters, 2005, 95, 136101.	2.9	176
66	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
67	Density-functional study ofCuatoms, monolayers, films, and coadsorbates on polarZnOsurfaces. Physical Review B, 2004, 69, .	1.1	85
68	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
69	Density-functional study of the structure and stability of ZnO surfaces. Physical Review B, 2003, 67, .	1.1	536
70	Ab initio analysis of electron energy loss spectra for complex oxides. Ultramicroscopy, 1999, 80, 145-151.	0.8	20
71	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