

Frank Stefan Tautz

List of Publications by Year in descending order

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165
papers

6,691
citations

61984

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69250

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173
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173
docs citations

173
times ranked

4802
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of high-resolution STM/AFM imaging with functionalized tips. <i>Physical Review B</i> , 2014, 90, .	3.2	438
2	Structure and bonding of large aromatic molecules on noble metal surfaces: The example of PTCDA. <i>Progress in Surface Science</i> , 2007, 82, 479-520.	8.3	349
3	Molecular Distortions and Chemical Bonding of a Large π -Conjugated Molecule on a Metal Surface. <i>Physical Review Letters</i> , 2005, 94, 036106.	7.8	258
4	Free-electron-like dispersion in an organic monolayer film on a metal substrate. <i>Nature</i> , 2006, 444, 350-353.	27.8	247
5	Understanding and tuning the epitaxy of large aromatic adsorbates by molecular design. <i>Nature</i> , 2003, 425, 602-605.	27.8	234
6	Structure and Energetics of Azobenzene on Ag(111): Benchmarking Semiempirical Dispersion Correction Approaches. <i>Physical Review Letters</i> , 2010, 104, 036102.	7.8	222
7	Origin of High-Resolution IETS-STM Images of Organic Molecules with Functionalized Tips. <i>Physical Review Letters</i> , 2014, 113, 226101.	7.8	165
8	A novel method achieving ultra-high geometrical resolution in scanning tunnelling microscopy. <i>New Journal of Physics</i> , 2008, 10, 053012.	2.9	158
9	Role of Intermolecular Interactions on the Electronic and Geometric Structure of a Large π -Conjugated Molecule Adsorbed on a Metal Surface. <i>Physical Review Letters</i> , 2008, 100, 136103.	7.8	147
10	Vertical bonding distances of PTCDA on Au(111) and Ag(111): Relation to the bonding type. <i>Surface Science</i> , 2007, 601, 1566-1573.	1.9	145
11	Adsorption structure and scanning tunneling data of a prototype organic-inorganic interface: PTCDA on Ag(111). <i>Physical Review B</i> , 2007, 76, .	3.2	136
12	Imaging Pauli Repulsion in Scanning Tunneling Microscopy. <i>Physical Review Letters</i> , 2010, 105, 086103.	7.8	135
13	Lateral adsorption geometry and site-specific electronic structure of a large organic chemisorbate on a metal surface. <i>Physical Review B</i> , 2006, 74, .	3.2	126
14	Kondo effect by controlled cleavage of a single-molecule contact. <i>Nanotechnology</i> , 2008, 19, 065401.	2.6	114
15	Direct Imaging of Intermolecular Bonds in Scanning Tunneling Microscopy. <i>Journal of the American Chemical Society</i> , 2010, 132, 11864-11865.	13.7	106
16	Single Molecule and Single Atom Sensors for Atomic Resolution Imaging of Chemically Complex Surfaces. <i>Journal of the American Chemical Society</i> , 2011, 133, 16847-16851.	13.7	104
17	The interplay between interface structure, energy level alignment and chemical bonding strength at organic-metal interfaces. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 1530-1548.	2.8	100
18	Orbital tomography: Deconvoluting photoemission spectra of organic molecules. <i>Physical Review B</i> , 2011, 84, .	3.2	99

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37	Ultimate resolution electron energy loss spectroscopy at H/Si(100) surfaces. Journal of Applied Physics, 1998, 84, 6636-6643.	2.5	54
38	Polycyclic aromates on close-packed metal surfaces: functionalization, molecular chemisorption and organic epitaxy. New Journal of Physics, 2004, 6, 4-4.	2.9	52
39	The nature of elementary excitations below and above the metamagnetic transition in CeRu ₂ Si ₂ . Physica B: Condensed Matter, 1995, 206-207, 29-32.	2.7	51
40	Adsorption height determination of nonequivalent C and O species of PTCDA on Ag(110) using x-ray standing waves. Physical Review B, 2013, 87, .	3.2	51
41	A chemically driven quantum phase transition in a two-molecule Kondo system. Nature Physics, 2016, 12, 867-873.	16.7	49
42	Orbital tomography for highly symmetric adsorbate systems. Europhysics Letters, 2012, 100, 26008.	2.0	45
43	Differences in vibronic and electronic excitations of PTCDA on Ag(111) and Ag(110). Surface Science, 2000, 454-456, 60-66.	1.9	43
44	Commensurate Registry and Chemisorption at a Hetero-organic Interface. Physical Review Letters, 2012, 108, 106103.	7.8	43
45	Quantification of finite-temperature effects on adsorption geometries of C_{60} -conjugated molecules: Azobenzene/Ag(111). Physical Review B, 2013, 88, .	3.2	43
46	Tracing orbital images on ultrafast time scales. Science, 2021, 371, 1056-1059.	12.6	42
47	A comparison of the chemisorption behaviour of PTCDA on different Ag surfaces. Surface Science, 2002, 502-503, 176-184.	1.9	41
48	A standing molecule as a single-electron field emitter. Nature, 2018, 558, 573-576.	27.8	41
49	Autonomous robotic nanofabrication with reinforcement learning. Science Advances, 2020, 6, .	10.3	40
50	Energy Ordering of Molecular Orbitals. Journal of Physical Chemistry Letters, 2017, 8, 208-213.	4.6	38
51	Electrical transport through a mechanically gated molecular wire. Physical Review B, 2011, 83, .	3.2	37
52	Energy offsets within a molecular monolayer: the influence of the molecular environment. New Journal of Physics, 2013, 15, 033017.	2.9	35
53	Quantum oscillation measurements of band magnetism in UPt ₃ and CeRu ₂ Si ₂ . Physica B: Condensed Matter, 1994, 199-200, 63-66.	2.7	33
54	Strong K-induced changes in perylene-tetracarboxylic-dianhydride films on Ag(110) studied by HREELS and LEED. Surface Science, 2001, 482-485, 1241-1248.	1.9	33

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55	Quantitative imaging of electric surface potentials with single-atom sensitivity. <i>Nature Materials</i> , 2019, 18, 853-859.	27.5	31
56	Kekulene: On-Surface Synthesis, Orbital Structure, and Aromatic Stabilization. <i>ACS Nano</i> , 2020, 14, 15766-15775.	14.6	30
57	Long Vertical Distance Bonding of the Hexagonal Boron Nitride Monolayer on the Cu(111) Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23964-23973.	3.1	29
58	Structure, bonding, and growth at a metal-organic interface in the weak chemisorption regime: Perylene-Ag(111). <i>Journal of Materials Research</i> , 2004, 19, 2028-2039.	2.6	28
59	Growth of pentacene on Ag(111) surface: A NEXAFS study. <i>Applied Surface Science</i> , 2007, 254, 103-107.	6.1	28
60	Modeling intermolecular interactions of physisorbed organic molecules using pair potential calculations. <i>Journal of Chemical Physics</i> , 2011, 135, 234703.	3.0	28
61	Site-Specific Polarization Screening in Organic Thin Films. <i>Physical Review Letters</i> , 2009, 102, 177405.	7.8	27
62	Structure and growth of tetracene on Ag(111). <i>Physical Review B</i> , 2011, 84, .	3.2	27
63	Substrate influence on the ordering of organic submonolayers: a comparative study of PTCDA on Ag(110) and Ag(111) using HREELS. <i>Applied Surface Science</i> , 2000, 166, 363-369.	6.1	26
64	Ab initio study of a mechanically gated molecule: From weak to strong correlation. <i>Physical Review B</i> , 2011, 84, .	3.2	26
65	Charge transfer and symmetry reduction at the CuPc/Ag(110) interface studied by photoemission tomography. <i>Physical Review B</i> , 2016, 94, .	3.2	25
66	Understanding the photoemission distribution of strongly interacting two-dimensional overlayers. <i>Physical Review B</i> , 2017, 96, .	3.2	25
67	Bulky spacer groups – A valid strategy to control the coupling of functional molecules to surfaces?. <i>Chemical Physics Letters</i> , 2010, 499, 247-249.	2.6	24
68	Transferring spin into an extended π -orbital of a large molecule. <i>Physical Review B</i> , 2015, 91, .	3.2	24
69	Modification of the PTCDA-Ag bond by forming a heteromolecular bilayer film. <i>Physical Review B</i> , 2015, 91, .	3.2	24
70	Patterning a hydrogen-bonded molecular monolayer with a hand-controlled scanning probe microscope. <i>Beilstein Journal of Nanotechnology</i> , 2014, 5, 1926-1932.	2.8	23
71	Reassessment of core-level photoemission spectra of reconstructed SiC(0001) surfaces. <i>Surface Science</i> , 2000, 470, L25-L31.	1.9	22
72	Controlling the growth of multiple ordered heteromolecular phases by utilizing intermolecular repulsion. <i>Nature Materials</i> , 2017, 16, 628-633.	27.5	22

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73	Non-dipolar effects in photoelectron-based normal incidence X-ray standing wave experiments. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2018, 222, 106-116.	1.7	22
74	On the decoupling of molecules at metal surfaces. <i>Chemical Communications</i> , 2018, 54, 9039-9042.	4.1	22
75	Calibrating atomic-scale force sensors installed at the tip apex of a scanning tunneling microscope. <i>Physical Review B</i> , 2013, 87, .	3.2	21
76	Surface plasmons at MOCVD-grown GaN. <i>Semiconductor Science and Technology</i> , 1998, 13, 1396-1400.	2.0	19
77	Adsorption height alignment at heteromolecular hybrid interfaces. <i>Physical Review B</i> , 2014, 89, .	3.2	19
78	Low vibration laboratory with a single-stage vibration isolation for microscopy applications. <i>Review of Scientific Instruments</i> , 2017, 88, 023703.	1.3	19
79	Quantum transport through STM-lifted single PTCDA molecules. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 93, 335-343.	2.3	18
80	Virtual reality visual feedback for hand-controlled scanning probe microscopy manipulation of single molecules. <i>Beilstein Journal of Nanotechnology</i> , 2015, 6, 2148-2153.	2.8	18
81	Identifying surface reaction intermediates with photoemission tomography. <i>Nature Communications</i> , 2019, 10, 3189.	12.8	18
82	Coexisting Charge States in a Unary Organic Monolayer Film on a Metal. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 6438-6445.	4.6	18
83	Neutron-diffraction study of antiferromagnetic order in U(Pt, Pd) ₃ . <i>Physica B: Condensed Matter</i> , 1997, 230-232, 49-52.	2.7	17
84	Switching orientation of adsorbed molecules: Reverse domino on a metal surface. <i>Surface Science</i> , 2016, 643, 98-107.	1.9	17
85	Torricelli: A software to determine atomic spatial distributions from normal incidence x-ray standing wave data. <i>Computer Physics Communications</i> , 2019, 235, 502-513.	7.5	17
86	Charge-Promoted Self-Metalation of Porphyrins on an Oxide Surface. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 5078-5082.	13.8	17
87	Structural, vibrational and electronic properties of faceted GaN (0001̄ _h) surfaces. <i>Surface Science</i> , 1999, 427-428, 250-256.	1.9	15
88	Strong dispersion of the surface optical phonon of silicon carbide in the near vicinity of the surface Brillouin zone center. <i>Surface Science</i> , 2006, 600, 2886-2893.	1.9	15
89	Electron Energy Loss of Terrylene Deposited on Au(111): Vibrational and Electronic Spectroscopy. <i>Journal of Physical Chemistry C</i> , 2015, 119, 277-283.	3.1	15
90	Tailoring metal-organic hybrid interfaces: heteromolecular structures with varying stoichiometry on Ag(111). <i>New Journal of Physics</i> , 2015, 17, 023046.	2.9	15

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91	Photoelectron spectroscopy at clean and hydrogenated $c(2\sqrt{3}\times 2)$ -SiC(100) surfaces. Applied Surface Science, 1998, 123-124, 17-21.	6.1	14
92	Electron energy loss spectroscopy with parallel readout of energy and momentum. Review of Scientific Instruments, 2017, 88, 033903.	1.3	14
93	In situ disentangling surface state transport channels of a topological insulator thin film by gating. Npj Quantum Materials, 2018, 3, .	5.2	14
94	Molecular Model of a Quantum Dot Beyond the Constant Interaction Approximation. Physical Review Letters, 2018, 120, 206801.	7.8	14
95	Resolving Ambiguity of the Kondo Temperature Determination in Mechanically Tunable Single-Molecule Kondo Systems. Journal of Physical Chemistry Letters, 2021, 12, 6320-6325.	4.6	14
96	Landau theory revisited. Ferroelectrics, 1992, 128, 255-264.	0.6	13
97	Polarity, Morphology and Reactivity of Epitaxial GaN Films on Al ₂ O ₃ (0001). Physica Status Solidi A, 2000, 177, 5-14.	1.7	13
98	Coverage-driven dissociation of azobenzene on Cu(111): a route towards defined surface functionalization. Chemical Communications, 2015, 51, 15324-15327.	4.1	13
99	Adsorption geometry and interface states: Relaxed and compressed phases of NTCDA/Ag(111). Physical Review B, 2016, 94, .	3.2	13
100	Determination of the adsorption geometry of PTCDA on the Cu(100) surface. Physical Review B, 2017, 96, .	3.2	13
101	Lateral scattering potential of the PTCDA/Ag(111) interface state. Physical Review B, 2018, 98, .	3.2	13
102	Surfactant-Mediated Epitaxial Growth of Single-Layer Graphene in an Unconventional Orientation on SiC. Physical Review Letters, 2020, 125, 106102.	7.8	13
103	kMap.py: A Python program for simulation and data analysis in photoemission tomography. Computer Physics Communications, 2021, 263, 107905.	7.5	13
104	Investigation of modified 3C SiC(100) surfaces by surface-sensitive techniques. Diamond and Related Materials, 1997, 6, 1353-1357.	3.9	12
105	Surface phonons of clean and hydrogen terminated Si(1 1 0) surfaces. Surface Science, 2005, 582, 159-172.	1.9	12
106	Dynamical bistability of single-molecule junctions: A combined experimental and theoretical study of PTCDA on Ag(111). Physical Review B, 2011, 84, .	3.2	12
107	The role of surface corrugation and tip oscillation in single-molecule manipulation with a non-contact atomic force microscope. Beilstein Journal of Nanotechnology, 2014, 5, 202-209.	2.8	12
108	The interplay between molecular orientation, film morphology and luminescence properties of tetracene thin films on epitaxial AlO _x /Ni ₃ Al(111). Surface Science, 2006, 600, 4679-4689.	1.9	11

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109	Spectral properties of a molecular wire in the Kondo regime. <i>Physica Status Solidi (B): Basic Research</i> , 2013, 250, 2386-2393.	1.5	11
110	Quantum interference effects in molecular spin hybrids. <i>Physical Review B</i> , 2017, 95, .	3.2	11
111	Coverage-dependent anisotropy of the NTCDA/Ag(111) interface state dispersion. <i>Physical Review B</i> , 2019, 100, .	3.2	11
112	Surface phonons of clean, hydrogen- and deuterium-terminated Si(001) surfaces. <i>Surface Science</i> , 2006, 600, 3446-3455.	1.9	9
113	Fundamental interface properties in OFETs: Bonding, structure and function of molecular adsorbate layers on solid surfaces. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2008, 205, 511-525.	1.8	9
114	Spontaneous Change in Molecular Orientation at Order-Disorder Transition of Tetracene on Ag(111). <i>Journal of Physical Chemistry C</i> , 2013, 117, 9212-9222.	3.1	9
115	X-ray standing wave simulations based on Fourier vector analysis as a method to retrieve complex molecular adsorption geometries. <i>Frontiers in Physics</i> , 2014, 2, .	2.1	9
116	Role of the Central Metal Atom in Substrate-Mediated Molecular Interactions in Phthalocyanine-Based Heteromolecular Monolayers. <i>Journal of Physical Chemistry C</i> , 2018, 122, 8491-8504.	3.1	9
117	Can photoemission tomography be useful for small, strongly-interacting adsorbate systems?. <i>New Journal of Physics</i> , 2019, 21, 043003.	2.9	9
118	Quantitative analysis of the electronic decoupling of an organic semiconductor molecule at a metal interface by a monolayer of hexagonal boron nitride. <i>Physical Review B</i> , 2019, 99, .	3.2	9
119	In-situ four-tip STM investigation of the transition from 2D to 3D charge transport in SrTiO ₃ . <i>Scientific Reports</i> , 2019, 9, 2476.	3.3	9
120	Room temperature in-situ measurement of the spin voltage of a BiSbTe ₃ thin film. <i>Scientific Reports</i> , 2020, 10, 2816.	3.3	9
121	Surface state-derived electronic transitions of SiC(001). <i>Surface Science</i> , 1999, 420, 87-94.	1.9	8
122	Tuning and probing interfacial bonding channels for a functionalized organic molecule by surface modification. <i>Physical Review B</i> , 2013, 87, .	3.2	8
123	Compact extreme ultraviolet source for laboratory-based photoemission spectromicroscopy. <i>Applied Physics Letters</i> , 2016, 108, .	3.3	8
124	Au enrichment and vertical relaxation of the Cu ₃ Au(111) surface studied by normal-incidence x-ray standing waves. <i>Physical Review B</i> , 2016, 93, .	3.2	8
125	Scanning quantum dot microscopy: A quantitative method to measure local electrostatic potential near surfaces. <i>Japanese Journal of Applied Physics</i> , 2016, 55, 08NA04.	1.5	8
126	Two-degree-of-freedom control combining machine learning and extremum seeking for fast scanning quantum dot microscopy. , 2018, , .		8

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127	A millikelvin scanning tunneling microscope in ultra-high vacuum with adiabatic demagnetization refrigeration. <i>Review of Scientific Instruments</i> , 2021, 92, 063701.	1.3	8
128	Reactivity and morphology of $(10\overline{12})$ -faceted and $(3\sqrt{3}\times 3)$ -reconstructed GaN(0001)bar epilayers grown on sapphire(0001). <i>Journal of Physics Condensed Matter</i> , 1999, 11, 8035-8048.	1.8	7
129	Control on a molecular scale: A perspective. , 2016, , .		7
130	Inelastic electron tunneling spectroscopy for probing strongly correlated many-body systems by scanning tunneling microscopy. <i>Physical Review B</i> , 2020, 101, .	3.2	7
131	Going beyond Pentacene: Photoemission Tomography of a Heptacene Monolayer on Ag(110). <i>Journal of Physical Chemistry C</i> , 2021, 125, 2918-2925.	3.1	7
132	Hexacene on Cu(110) and Ag(110): Influence of the Substrate on Molecular Orientation and Interfacial Charge Transfer. <i>Journal of Physical Chemistry C</i> , 2022, 126, 5036-5045.	3.1	7
133	Collective Surface Excitations in 3C-SiC(100). <i>Materials Science Forum</i> , 1998, 264-268, 347-350.	0.3	6
134	Bonding and vibrational dynamics of a large π -conjugated molecule on a metal surface. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 224010.	1.8	6
135	Focal-Series Reconstruction in Low-Energy Electron Microscopy. <i>Microscopy and Microanalysis</i> , 2014, 20, 968-973.	0.4	6
136	Controlling the electronic and physical coupling on dielectric thin films. <i>Beilstein Journal of Nanotechnology</i> , 2020, 11, 1492-1503.	2.8	6
137	Lifting the Spin-Momentum Locking in Ultra-Thin Topological Insulator Films. <i>Advanced Quantum Technologies</i> , 2021, 4, 2100083.	3.9	6
138	Transformation of metallic boron into substitutional dopants in graphene on $6H\sqrt{3}\times\sqrt{3}$ -SiC(0001). <i>Physical Review B</i> , 2016, 93, .	3.2	5
139	The theory of scanning quantum dot microscopy. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 475901.	1.8	5
140	Momentum microscopy on the micrometer scale: photoemission micro-tomography applied to single molecular domains. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 114003.	1.8	5
141	Parasitic conduction channels in topological insulator thin films. <i>Physical Review B</i> , 2020, 101, .	3.2	5
142	Vertical position of Sr dopants in the $\sqrt{2}\times\sqrt{2}$ superconductor. <i>Physical Review B</i> , 2021, 104, .	3.2	5
143	The stabilization potential of a standing molecule. <i>Science Advances</i> , 2021, 7, eabj9751.	10.3	5
144	Molecular Flexibility as a Factor Affecting the Surface Ordering of Organic Adsorbates on Metal Substrates. <i>Langmuir</i> , 2006, 22, 9572-9579.	3.5	4

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145	Comment on "Electron Core-Hole Interaction and Its Induced Ionic Structural Relaxation in Molecular Systems under X-Ray Irradiation", Physical Review Letters, 2007, 99, 059601; discussion 059602.	7.8	4
146	Surface structures of tellurium on Si(111)-(7 \times 7) studied by low-energy electron diffraction and scanning tunneling microscopy. Surface Science, 2019, 681, 130-133.	1.9	4
147	Hydrogen On Semiconductor Surfaces. Materials Research Society Symposia Proceedings, 1998, 513, 3.	0.1	3
148	Direct Evidence of the Temperature-Induced Molecular Reorientation in Tetracene Thin Films on AlO _x /Ni ₃ Al(111). Journal of Physical Chemistry C, 2014, 118, 22678-22682.	3.1	3
149	Hand Controlled Manipulation of Single Molecules via a Scanning Probe Microscope with a 3D Virtual Reality Interface. Journal of Visualized Experiments, 2016, , .	0.3	3
150	Adsorption-induced symmetry reduction of metal-phthalocyanines studied by vibrational spectroscopy. Physical Review B, 2017, 96, .	3.2	3
151	Dependence of the adsorption height of graphenelike adsorbates on their dimensionality. Physical Review B, 2018, 98, .	3.2	3
152	Ladungsunterstützte Selbstmetallierung von Porphyrinen auf Oxidoberflächen. Angewandte Chemie, 2021, 133, 5138-5142.	2.0	3
153	The magnetic phase diagram of UPt ₃ alloyed with Pd. Physica B: Condensed Matter, 1996, 223-224, 178-180.	2.7	2
154	A Comparative Study of a Triphenylene Tricarbonyl Chromium Complex and Its Uncoordinated Arene Ligand on the Ag(111) Surface: Influence of the Complexation on the Adsorption. Journal of Physical Chemistry C, 2009, 113, 6014-6021.	3.1	2
155	Adsorption of 3,4,9,10-Perylenetetracarboxylic Acid Dianhydride on the Cu ₃ Au(111) Surface Studied by Normal-Incidence X-ray Standing Waves. Journal of Physical Chemistry C, 2018, 122, 10904-10917.	3.1	2
156	Perspectives of Molecular Manipulation and Fabrication. Advances in Atom and Single Molecule Machines, 2017, , 253-319.	0.0	2
157	Design Principles for Metastable Standing Molecules. Journal of Physical Chemistry C, 2022, 126, 6880-6891.	3.1	2
158	Low energy excitations of highly correlated electron systems. Journal of Low Temperature Physics, 1994, 95, 39-43.	1.4	1
159	Scanning Tunnelling Microscopy with Single Molecule Force Sensors. Nanoscience and Technology, 2015, , 275-301.	1.5	1
160	Nanoscale tip positioning with a multi-tip scanning tunneling microscope using topography images. Review of Scientific Instruments, 2022, 93, 013702.	1.3	1
161	Boron nitride on SiC(0001). Physical Review Materials, 2022, 6, .	2.4	1
162	Fundamental Interface Properties in OFETs: Bonding, Structure and Function of Molecular Adsorbate Layers on Solid Surfaces. , 0, , 235-262.		0

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163	Manipulation on a molecular level: towards controlled molecular 3D printing. , 2016, , .		0
164	Elektronenorbitale in 3D. Physik in Unserer Zeit, 2016, 47, 192-198.	0.0	0
165	A standing molecule as a coherent single-electron field emitter. , 2021, , .		0