Sibylle Gemming

List of Publications by Year
in descending order

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157	4,175	147801	133252
papers	citations	31 h-index	59 g-index

162	162	162	6112
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum transport and microwave scattering on fractal lattices. Zeitschrift Fur Kristallographie - Crystalline Materials, 2022, 237, 179-190.	0.8	1
2	Deposition of Nanosized Amino Acid Functionalized Bismuth Oxido Clusters on Gold Surfaces. Nanomaterials, 2022, 12, 1815.	4.1	1
3	Organogels from Diketopyrrolopyrrole Copolymer Ionene/Polythiophene Blends Exhibit Ground-State Single Electron Transfer in the Solid State. Macromolecules, 2022, 55, 4979-4994.	4.8	2
4	Controlling excitons in the quantum tunneling regime in a hybrid plasmonic/2D semiconductor interface. Applied Physics Reviews, 2022, 9, 031401.	11.3	6
5	Electron Mobility of Diketopyrrolopyrrole Copolymers Is Robust against Homocoupling Defects. Chemistry of Materials, 2021, 33, 668-677.	6.7	11
6	Hydrogen Bonds Control Single-Chain Conformation, Crystallinity, and Electron Transport in Isoelectronic Diketopyrrolopyrrole Copolymers. Chemistry of Materials, 2021, 33, 2635-2645.	6.7	23
7	Localization of edge states at triangular defects in periodic <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> monolayers. Physical Review Materials, 2021, 5, .	2.4	3
8	Interactions of Ruddlesden-Popper Phases and Migration-Induced Field-Stabilized Polar Phase in Strontium Titanate. Crystals, 2021, 11, 693.	2.2	2
9	Theoretical evidence for the Peierls transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>NbO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2021, 104, .	3.2	6
10	Singleâ€Molecule Doping: Conductance Changed By Transition Metal Centers in Salen Molecules. Advanced Electronic Materials, 2021, 7, 2100252.	5.1	5
11	Describing chain-like assembly of ethoxygroup-functionalized organic molecules on Au(111) using high-throughput simulations. Scientific Reports, 2021, 11, 14649.	3.3	1
12	Formation, structure, and optical properties of copper chromite thin films for high-temperature solar absorbers. Materialia, 2021, 18, 101156.	2.7	4
13	Closedâ€Loop Defect States in 2D Materials with Honeycomb Lattice Structure: Molybdenum Disulfide. Physica Status Solidi (B): Basic Research, 2021, 258, 2100214.	1.5	0
14	A combined experimental and theoretical study of 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene adsorption on Au(111). Surface Science, 2021, 712, 121877.	1.9	4
15	Observation of Roomâ€Temperature Dark Exciton Emission in Nanopatchâ€Decorated Monolayer WSe₂ on Metal Substrate. Advanced Optical Materials, 2021, 9, 2101801.	7.3	11
16	Directionality of metal-induced crystallization and layer exchange in amorphous carbon/nickel thin film stacks. Carbon, 2020, 159, 656-667.	10.3	7
17	A correlation study of layer growth rate, thickness uniformity, stoichiometry, and hydrogen impurity level in HfO2 thin films grown by ALD between <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si60.svg"><mml:mrow><mml:mn>100</mml:mn><mml:mspace width="0.25em" /><mml:mi>Â°</mml:mi><mml:mtext>C</mml:mtext></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si61.svg"><mml:mrow><mml:mn>350</mml:mn></mml:mrow>	6.1	35
18	Formation and crystallographic orientation of NiSi2â€“Si interfaces. Journal of Applied Physics, 2020, 128, 085301.	2.5	7

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19	Topological Hall Effect in Single Thick SrRuO₃ Layers Induced by Defect Engineering. Advanced Electronic Materials, 2020, 6, 2000184.	5.1	24
20	Tunable Magnetic Vortex Dynamics in Ion-Implanted Permalloy Disks. ACS Applied Materials & Interfaces, 2020, 12, 27812-27818.	8.0	8
21	Anisotropy of colloidal components propels field-activated stirrers and movers. Physical Review Research, 2020, 2, .	3.6	6
22	Autocorrected off-axis holography of two-dimensional materials. Physical Review Research, 2020, 2, .	3.6	5
23	Electron transport through NiSi₂â€“Si contacts and their role in reconfigurable field-effect transistors. Journal of Physics Condensed Matter, 2019, 31, 355002.	1.8	7
24	Field-responsive colloidal assemblies defined by magnetic anisotropy. Physical Review E, 2019, 100, 012608.	2.1	11
25	Towards Reconfigurable Electronics: Silicidation of Top-Down Fabricated Silicon Nanowires. Applied Sciences (Switzerland), 2019, 9, 3462.	2.5	16
26	A Twoâ€Parameter Model for Colloidal Particles with an Extended Magnetic Cap. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1900506.	1.8	2
27	Direct Correction of Residual Symmetric Aberrations in Electron Holograms of Weak Phase Objects. Microscopy and Microanalysis, 2019, 25, 98-99.	0.4	1
28	Transparent conductive tantalum doped tin oxide as selectively solar-transmitting coating for high temperature solar thermal applications. Solar Energy Materials and Solar Cells, 2019, 196, 84-93.	6.2	19
29	Probing interlayer excitons in a vertical van der Waals p-n junction using a scanning probe microscopy technique. Journal of Physics Condensed Matter, 2019, 31, 114001.	1.8	6
30	Radially resolved electronic structure and charge carrier transport in silicon nanowires. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 108, 181-186.	2.7	6
31	Feasible Device Architectures for Ultrascaled CNTFETs. IEEE Nanotechnology Magazine, 2018, 17, 100-107.	2.0	14
32	Dynamical universality classes of simple growth and lattice gas models. Journal of Physics A: Mathematical and Theoretical, 2018, 51, 035003.	2.1	9
33	Percolated Si:SiO2 Nanocomposites: Oven- vs. Millisecond Laser-Induced Crystallization of SiOx Thin Films. Nanomaterials, 2018, 8, 525.	4.1	6
34	Functional thiols as repair and doping agents of defective MoS₂ monolayers. Journal of Physics Condensed Matter, 2018, 30, 235302.	1.8	8
35	Cluster Tool for In Situ Processing and Comprehensive Characterization of Thin Films at High Temperatures. Analytical Chemistry, 2018, 90, 7837-7842.	6.5	5
36	Enhancing the magnetic moment of ferrimagnetic NiCo2O4 via ion irradiation driven oxygen vacancies. APL Materials, 2018, 6, .	5.1	21

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37	Tuning the conductance of a molecular wire by the interplay of donor and acceptor units. Nanoscale, 2018, 10, 17131-17139.	5.6	4
38	Analysis of the defect clusters in congruent lithium tantalate. Physical Review Materials, 2018, 2, .	2.4	18
39	Molecular Doping of a High Mobility Diketopyrrolopyrroleâ€“Dithienylthieno[3,2-b]thiophene Donorâ€“Acceptor Copolymer with F6TCNNQ. Macromolecules, 2017, 50, 914-926.	4.8	66
40	Local scale-invariance of the 2â€‰â€‰+â€‰â€‰1 dimensional Kardarâ€“Parisiâ€“Zhang model. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 12LT01.	2.1	5
41	Influence of Electric Fields on the Electron Transport in Donorâ€“Acceptor Polymers. Journal of Physical Chemistry C, 2017, 121, 3714-3723.	3.1	7
42	Chemical and Electronic Repair Mechanism of Defects in MoS₂ Monolayers. ACS Nano, 2017, 11, 9989-9996.	14.6	80
43	Influence of Nickel Catalyst Morphology on Layer-Exchange-Based Carbon Crystallisation of Ni/a-C Bilayers. Physica Status Solidi (B): Basic Research, 2017, 254, 1700234.	1.5	5
44	Suppressing correlations in massively parallel simulations of lattice models. Computer Physics Communications, 2017, 220, 205-211.	7.5	4
45	Phase Transitions in C:Ni Nanocomposite Templates during Diameterâ€Selective CVD Synthesis of SWCNTs. Physica Status Solidi (B): Basic Research, 2017, 254, 1700228.	1.5	1
46	Elastic and piezoresistive properties of nickel carbides from first principles. Physical Review B, 2017, 95, .	3.2	8
47	Structure variations within certain rare earth disilicides. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C287-C287.	0.1	0
48	Theoretical investigation of in situ k-restore processes for damaged ultra-low-k dielectrics. Microelectronic Engineering, 2016, 156, 121-125.	2.4	1
49	Hopping-Based Charge Transfer in Diketopyrrolopyrrole-Based Donorâ€“Acceptor Polymers: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 9581-9587.	3.1	11
50	Universality of (2+1)-dimensional restricted solid-on-solid models. Physical Review E, 2016, 94, 022107.	2.1	17
51	Carbonâ€‰:â€‰nickel nanocomposite templates â€“ predefined stable catalysts for diameter-controlled growth of single-walled carbon nanotubes. Nanoscale, 2016, 8, 14888-14897.	5.6	10
52	Non-equilibrium dynamics of magnetically anisotropic particles under oscillating fields. European Physical Journal E, 2016, 39, 69.	1.6	19
53	Bit-vectorized GPU implementation of a stochastic cellular automaton model for surface growth. , 2016, , .		1
54	Comparison of atomistic quantum transport and numerical device simulation for carbon nanotube field-effect transistors. , 2016, , .		3

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55	Rotational friction of dipolar colloids measured by driven torsional oscillations. Scientific Reports, 2016, 6, 34193.	3.3	3
56	Thermally induced formation of metastable nanocomposites in amorphous Cr-Zr-O thin films deposited using reactive ion beam sputtering. Thin Solid Films, 2016, 612, 430-436.	1.8	9
57	High Conductivity in Molecularly pâ€Doped Diketopyrrolopyrroleâ€Based Polymer: The Impact of a High Dopant Strength and Good Structural Order. Advanced Materials, 2016, 28, 6003-6010.	21.0	130
58	Nickel-enhanced graphitic ordering of carbon ad-atoms during physical vapor deposition. Carbon, 2016, 100, 656-663.	10.3	19
59	Defect-induced magnetism in SiC: Interplay between ferromagnetism and paramagnetism. Physical Review B, 2015, 92, .	3.2	31
60	Theoretical investigation of an in situ k-restore process for damaged ultra-low-k materials based on plasma enhanced fragmentation. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2015, 33, 052203.	1.2	3
61	Theoretical investigation of in situ k-restore processes for damaged ultra-low-k materials. , 2015, , .		1
62	Stoichiometry variation for the atomic layer deposition of SrxTiyOz from Sr(iPr3Cp)2, Ti[N(CH3)2]4 and H2O. Thin Solid Films, 2015, 577, 134-142.	1.8	4
63	Lightâ€Induced Switching of Tunable Singleâ€Molecule Junctions. Advanced Science, 2015, 2, 1500017.	11.2	48
64	Carbon p Electron Ferromagnetism in Silicon Carbide. Scientific Reports, 2015, 5, 8999.	3.3	38
65	Optics, Mechanics, and Energetics of Two-Dimensional MoS₂ Nanostructures from a Theoretical Perspective. Accounts of Chemical Research, 2015, 48, 48-55.	15.6	53
66	Defect-induced magnetism in graphite through neutron irradiation. Physical Review B, 2014, 90, .	3.2	21
67	Compositionally modulated ripples during composite film growth: Three-dimensional pattern formation at the nanoscale. Physical Review B, 2014, 89, .	3.2	12
68	Aging of the (2+1)-dimensional Kardar-Parisi-Zhang model. Physical Review E, 2014, 89, 032146.	2.1	20
69	Microstructural Studies of Fluorineâ€<scp>I</scp>mplanted Titanium Aluminides for Enhanced Environmental Durability. Advanced Engineering Materials, 2014, 16, 52-59.	3.5	7
70	Probing a crystal's shortâ€range structure and local orbitals by Resonant Xâ€ray Diffraction methods. Crystal Research and Technology, 2014, 49, 43-54.	1.3	21
71	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. Tribology Letters, 2014, 53, 119-126.	2.6	89
72	Tetrahedral Amorphous Carbon Coatings for Friction Reduction of the Valve Train in Internal Combustion Engines. Advanced Engineering Materials, 2014, 16, 1226-1233.	3.5	12

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73	Disentangling defect-induced ferromagnetism in SiC. Physical Review B, 2014, 89, .	3.2	25
74	Surface-near modifications of SrTiO3 local symmetry due to nitrogen implantation investigated by grazing incidence XANES. Scripta Materialia, 2014, 86, 1-4.	5.2	9
75	Strontium titanate: An all-in-one rechargeable energy storage material. Journal of Power Sources, 2014, 267, 700-705.	7.8	23
76	Migration-induced field-stabilized polar phase in strontium titanate single crystals at room temperature. Physical Review B, 2013, 88, .	3.2	50
77	Resistive switching in thermally oxidized titanium films. , 2013, , .		1
78	Theoretical study on the CHâ‹¯NC hydrogen bond interaction in thiophene-based molecules. Computational and Theoretical Chemistry, 2013, 1005, 45-52.	2.5	5
79	Effects of the TiO2 buffer thickness on SrTiO3 (111) epitaxial films grown on GaN (0002). Journal of Applied Physics, 2013, 113, 154103.	2.5	5
80	Topology and Origin of Effective Spin Meron Pairs in Ferromagnetic Multilayer Elements. Physical Review Letters, 2013, 110, 177201.	7.8	55
81	DFT Investigation of the Heterostructure GaP(001) on Si(001). Nanoscience and Nanotechnology Letters, 2013, 5, 73-77.	0.4	5
82	Structure, Optical and Mechanical Properties of Direct Current Magnetron Sputtered Carbon: Vanadium Nanocomposite Thin Films. Nanoscience and Nanotechnology Letters, 2013, 5, 94-100.	0.4	3
83	Tilting of carbon encapsulated metallic nanocolumns in carbon-nickel nanocomposite films by ion beam assisted deposition. Applied Physics Letters, 2012, 101, 053112.	3.3	11
84	SWCNT growth from C:Ni nanocomposites. Physica Status Solidi (B): Basic Research, 2012, 249, 2357-2360.	1.5	5
85	Band gap tuning of carbon nanotubes for sensor and interconnect applications — A quantum simulation study. , 2012, , .		1
86	Environment Controlled Dewetting of Rhâ€“Pd Bilayers: A Route for Coreâ€“Shell Nanostructure Synthesis. Journal of Physical Chemistry C, 2012, 116, 14401-14407.	3.1	6
87	Nitrogen interstitial diffusion induced decomposition in AISI 304L austenitic stainless steel. Acta Materialia, 2012, 60, 4065-4076.	7.9	76
88	Conformational Analysis of Aqueous BMP-2 Using Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 1122-1130.	2.6	23
89	Phase Segregation and Transformations in Arsenic-Implanted ZnO Thin Films. Journal of Physical Chemistry C, 2011, 115, 8798-8807.	3.1	1
90	Crystallographic superstructure in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>R</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>PdSi<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow		

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91	Tribological Aspects of Carbon-Based Nanocoatings â€“ Theory and Simulation. Zeitschrift Fur Physikalische Chemie, 2011, 225, 379-387.	2.8	4
92	High resolution TEM study of WS₂ nanotubes. Physica Status Solidi (B): Basic Research, 2011, 248, 2716-2719.	1.5	35
93	Back Cover: High resolution TEM study of WS₂ nanotubes (Phys. Status Solidi B 11/2011). Physica Status Solidi (B): Basic Research, 2011, 248, .	1.5	0
94	Low-temperature modeling for degenerate and frustrated Heisenberg systems with anisotropy. Computer Physics Communications, 2010, 181, 806-812.	7.5	2
95	Molecular dynamics simulations of BMPâ€2 adsorption on a hydrophobic surface. Materialwissenschaft Und Werkstofftechnik, 2010, 41, 1048-1053.	0.9	15
96	Surface modeling and chemical solution deposition of SrO(SrTiO3) Ruddlesdenâ€“Popper phases. Acta Materialia, 2010, 58, 4650-4659.	7.9	20
97	Transition metal sulfide clusters below the clusterâ€“platelet transition: Theory and experiment. Physica Status Solidi (B): Basic Research, 2010, 247, 1069-1076.	1.5	17
98	Adsorption of nucleotides on the rutile (110) surface. International Journal of Materials Research, 2010, 101, 758-764.	0.3	22
99	Correlation of structure and conductance in nanowires. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s155-s155.	0.3	0
100	XRD, XAS and DFT study of the multiferroic mixed-valence compound YMn2O5. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, s39-s40.	0.3	0
101	Conduction at domain walls in oxide multiferroics. Nature Materials, 2009, 8, 229-234.	27.5	1,212
102	Two-scale modeling of adsorption processes at structured surfaces. Physica D: Nonlinear Phenomena, 2009, 238, 117-125.	2.8	6
103	One-dimensional (Mo3S3)n clusters: Building blocks of clusters materials and ideal nanowires for molecular electronics. Chemical Physics Letters, 2009, 474, 127-131.	2.6	13
104	Elastic properties and electronic structure of vanadium silicides-a density functional investigation. Acta Materialia, 2009, 57, 50-55.	7.9	19
105	Binding properties between ferroic oxides and metals. European Physical Journal B, 2009, 67, 57-62.	1.5	1
106	DFT modelling of defects in strontium titanate. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s208-s209.	0.3	0
107	Reversible structural changes by electrostatic fields in strontium titanate at room temperature. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s232-s232.	0.3	0
108	Starâ€Shaped Oligobenzoates: Nonâ€conventional Mesogens Forming Columnar Helical Mesophases. Chemistry - A European Journal, 2008, 14, 3562-3576.	3.3	72

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109	Reduction of surface coverage of finite systems due to geometrical steps. European Physical Journal B, 2008, 62, 311-317.	1.5	0
110	Ab-initio calculation of exchange interactions in YMnO3. Computational Materials Science, 2008, 44, 79-81.	3.0	15
111	Atomic-Scale Structure of Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 3928-3931.	9.1	68
112	Current without external bias and diode effect in shuttling transport of nanoshafts. New Journal of Physics, 2008, 10, 103014.	2.9	5
113	Electromechanical Switch Based on Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 4093-4097.	9.1	45
114	Polymorphism in liquid crystals from star-shaped mesogens. Philosophical Magazine Letters, 2007, 87, 883-891.	1.2	8
115	Structural and electronic properties ofMo6S8clusters deposited on a Au(111) surface investigated with density functional theory. Physical Review B, 2007, 75, .	3.2	11
116	Structure and Stability of Molybdenum Sulfide Fullerenes. Angewandte Chemie - International Edition, 2007, 46, 623-627.	13.8	84
117	Curvature effects of nitrogen on graphitic sheets: Structures and energetics. Chemical Physics Letters, 2007, 447, 115-120.	2.6	32
118	TiSi₂ nanostructures â€“ enhanced conductivity at nanoscale?. Physica Status Solidi (B): Basic Research, 2007, 244, 3593-3600.	1.5	8
119	Catalysts on the edge. Nature Nanotechnology, 2007, 2, 21-22.	31.5	23
120	Simulation of Inorganic Nanotubes. Springer Series in Materials Science, 2007, , 33-57.	0.6	26
121	DNA-wrapped carbon nanotubes. Nanotechnology, 2007, 18, 245702.	2.6	88
122	Modelling ferroic functional elements. Journal of Computer-Aided Materials Design, 2007, 14, 211-218.	0.7	6
123	Theoretical Investigation of Interfaces. Springer Series in Materials Science, 2007, , 91-122.	0.6	2
124	MonS2n+x clustersâ€”magic numbers and platelets. Computational Materials Science, 2006, 35, 316-320.	3.0	29
125	Structure, stability and electronic properties of composite Mo1â€“xNbxS2 nanotubes. Physica Status Solidi (B): Basic Research, 2006, 243, 1757-1764.	1.5	46
126	Li doped Mo6S6 nanowires: elastic and electronic properties. Physica Status Solidi (B): Basic Research, 2006, 243, 3320-3324.	1.5	17

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127	SrTiO3(001)â^£LaAlO3(001) multilayers: A density-functional investigation. Acta Materialia, 2006, 54, 4299-4306.	7.9	36
128	Nanoplatelets made from MoS2 and WS2. Chemical Physics Letters, 2006, 418, 36-39.	2.6	49
129	C28fulleritesâ€”structure, electronic properties and intercalates. Physical Chemistry Chemical Physics, 2006, 8, 3320-3325.	2.8	31
130	Electronic and geometric structures of MoxSy and WxSy (x =1, 2, 4; y =1â€“12) clusters. Applied Physics A: Materials Science and Processing, 2006, 82, 161-166.	2.3	28
131	Density-functional study of Mo4S6 on Au(111). Applied Physics A: Materials Science and Processing, 2006, 82, 175-179.	2.3	7
132	Impurity and vacancy clustering at the Î£3(111)[1â^10] grain boundary in strontium titanate. Chemical Physics, 2005, 309, 3-13.	1.9	15
133	Electron microscopy, spectroscopy, and first-principles calculations of Cs2O. Journal of Solid State Chemistry, 2005, 178, 1190-1196.	2.9	14
134	Density-functional investigation of alloyed metallic nanowires. Computer Physics Communications, 2005, 169, 57-59.	7.5	4
135	Semi-flexible star-shaped molecules: conformational analysis of nano-segregated mesogens forming columnar liquid-crystal phases. International Journal of Materials Research, 2005, 96, 988-997.	0.8	9
136	Density-functional-based molecular-dynamics simulations of molten salts. Journal of Chemical Physics, 2005, 123, 134510.	3.0	23
137	Electronic structure ofGa84cluster compounds. Physical Review B, 2004, 70, .	3.2	15
138	Molecular Dynamics. ChemInform, 2004, 35, no.	0.0	0
139	Tunable discotic building blocks for liquid crystalline displays. Journal of Luminescence, 2004, 108, 143-147.	3.1	12
140	Synthesis of NiCl2 nanotubes and fullerene-like structures by laser ablation: theoretical considerations and comparison with MoS2 nanotubes. Physical Chemistry Chemical Physics, 2003, 5, 1644-1651.	2.8	48
141	Evidence for high negative charge densities in AlF3 coatings on oxidized silicon: a promising source for large drift fields. Physica E: Low-Dimensional Systems and Nanostructures, 2002, 14, 259-262.	2.7	8
142	Oxidative corrosion of adhesive interlayers. Physical Chemistry Chemical Physics, 2001, 3, 5140-5144.	2.8	3
143	Success and limits of common final-state approximations. Ultramicroscopy, 2001, 86, 319-324.	1.9	8
144	Core-hole effect in the ELNES of Î±-Al2O3: experiment and theory. Ultramicroscopy, 2001, 86, 339-342.	1.9	29

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145	Validity of the dipole-selection rule for the Al-L2,3 edge of Î±-Al2O3 under channeling conditions. Ultramicroscopy, 2001, 88, 253-263.	1.9	9
146	Density functional study of the Î£3 (111) [1bar10] symmetrical tilt grain boundary in SrTiO3. Journal of Physics Condensed Matter, 2001, 13, 3949-3960.	1.8	44
147	Microscopic structure and bonding at the Pd/SrTiO3 (001) Interface an ab-initio local-density-functional study. Integrated Ferroelectrics, 2001, 32, 267-278.	0.7	40
148	Ab initiocalculation of near-edge structures in electron-energy-loss spectra for metal-oxide crystals. Physical Review B, 1999, 60, 14025-14034.	3.2	58
149	Ab initio analysis of electron energy loss spectra for complex oxides. Ultramicroscopy, 1999, 80, 145-151.	1.9	20
150	Olefin Epoxidation by Methyltrioxorhenium: A Density Functional Study on Energetics and Mechanisms. Angewandte Chemie - International Edition, 1998, 37, 2211-2214.	13.8	70
151	A Density Functional Study of Interactions at the Metalâ€“Ceramic Interfaces Al/MgAl2O4 and Ag/MgAl2O4. Physica Status Solidi A, 1998, 166, 417-428.	1.7	25
152	Lewis Acidity and Reactivity of Transition Metal Oxo Complexes. A Comparative Density Functional Study of CH3ReO3, CH3TcO3, and Their Base Adducts. Organometallics, 1997, 16, 1786-1792.	2.3	26
153	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. Journal of the American Chemical Society, 1997, 119, 3159-3160.	13.7	43
154	Density Functional Study on the Electronic Structure of Trioxorhenium Organyls. Organometallics, 1996, 15, 1872-1878.	2.3	32
155	Structure and properties of dimer, trimer and tetramer aggregates of methyltrioxorhenium (MTO): an ab initio study. Journal of Organometallic Chemistry, 1996, 514, 111-117.	1.8	15
156	The adsorption of CO on : a joint experimental and theoretical study. Surface Science, 1995, 330, 156-172.	1.9	24
157	An intermediate neglect of differential overlap technique for actinide compounds. Journal of Chemical Physics, 1994, 100, 1353-1365.	3.0	42