

Sibylle Gemming

List of Publications by Year in descending order

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157
papers

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147801

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162
docs citations

162
times ranked

6112
citing authors

#	ARTICLE	IF	CITATIONS
1	Conduction at domain walls in oxide multiferroics. <i>Nature Materials</i> , 2009, 8, 229-234.	27.5	1,212
2	High Conductivity in Molecularly p-doped Diketopyrrolopyrrole-Based Polymer: The Impact of a High Dopant Strength and Good Structural Order. <i>Advanced Materials</i> , 2016, 28, 6003-6010.	21.0	130
3	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. <i>Tribology Letters</i> , 2014, 53, 119-126.	2.6	89
4	DNA-wrapped carbon nanotubes. <i>Nanotechnology</i> , 2007, 18, 245702.	2.6	88
5	Structure and Stability of Molybdenum Sulfide Fullerenes. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 623-627.	13.8	84
6	Chemical and Electronic Repair Mechanism of Defects in MoS ₂ Monolayers. <i>ACS Nano</i> , 2017, 11, 9989-9996.	14.6	80
7	Nitrogen interstitial diffusion induced decomposition in AISI 304L austenitic stainless steel. <i>Acta Materialia</i> , 2012, 60, 4065-4076.	7.9	76
8	Star-Shaped Oligobenzoates: Non-conventional Mesogens Forming Columnar Helical Mesophases. <i>Chemistry - A European Journal</i> , 2008, 14, 3562-3576.	3.3	72
9	Olefin Epoxidation by Methyltrioxorhenium: A Density Functional Study on Energetics and Mechanisms. <i>Angewandte Chemie - International Edition</i> , 1998, 37, 2211-2214.	13.8	70
10	Atomic-Scale Structure of Mo ₆ S ₆ Nanowires. <i>Nano Letters</i> , 2008, 8, 3928-3931.	9.1	68
11	Molecular Doping of a High Mobility Diketopyrrolopyrrole-Dithienylthieno[3,2-b]thiophene Donor-Acceptor Copolymer with F6TCNNQ. <i>Macromolecules</i> , 2017, 50, 914-926.	4.8	66
12	Ab initio calculation of near-edge structures in electron-energy-loss spectra for metal-oxide crystals. <i>Physical Review B</i> , 1999, 60, 14025-14034.	3.2	58
13	Topology and Origin of Effective Spin Meron Pairs in Ferromagnetic Multilayer Elements. <i>Physical Review Letters</i> , 2013, 110, 177201.	7.8	55
14	Optics, Mechanics, and Energetics of Two-Dimensional MoS ₂ Nanostructures from a Theoretical Perspective. <i>Accounts of Chemical Research</i> , 2015, 48, 48-55.	15.6	53
15	Migration-induced field-stabilized polar phase in strontium titanate single crystals at room temperature. <i>Physical Review B</i> , 2013, 88, .	3.2	50
16	Nanoplatelets made from MoS ₂ and WS ₂ . <i>Chemical Physics Letters</i> , 2006, 418, 36-39.	2.6	49
17	Synthesis of NiCl ₂ nanotubes and fullerene-like structures by laser ablation: theoretical considerations and comparison with MoS ₂ nanotubes. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 1644-1651.	2.8	48
18	Light-Induced Switching of Tunable Single-Molecule Junctions. <i>Advanced Science</i> , 2015, 2, 1500017.	11.2	48

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37	Lewis Acidity and Reactivity of Transition Metal Oxo Complexes. A Comparative Density Functional Study of CH ₃ ReO ₃ , CH ₃ TcO ₃ , and Their Base Adducts. <i>Organometallics</i> , 1997, 16, 1786-1792.	2.3	26
38	Simulation of Inorganic Nanotubes. <i>Springer Series in Materials Science</i> , 2007, , 33-57.	0.6	26
39	A Density Functional Study of Interactions at the Metal–Ceramic Interfaces Al/MgAl ₂ O ₄ and Ag/MgAl ₂ O ₄ . <i>Physica Status Solidi A</i> , 1998, 166, 417-428.	1.7	25
40	Disentangling defect-induced ferromagnetism in SiC. <i>Physical Review B</i> , 2014, 89, .	3.2	25
41	The adsorption of CO on : a joint experimental and theoretical study. <i>Surface Science</i> , 1995, 330, 156-172.	1.9	24
42	Topological Hall Effect in Single Thick SrRuO ₃ Layers Induced by Defect Engineering. <i>Advanced Electronic Materials</i> , 2020, 6, 2000184.	5.1	24
43	Density-functional-based molecular-dynamics simulations of molten salts. <i>Journal of Chemical Physics</i> , 2005, 123, 134510.	3.0	23
44	Catalysts on the edge. <i>Nature Nanotechnology</i> , 2007, 2, 21-22.	31.5	23
45	Conformational Analysis of Aqueous BMP-2 Using Atomistic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1122-1130.	2.6	23
46	Strontium titanate: An all-in-one rechargeable energy storage material. <i>Journal of Power Sources</i> , 2014, 267, 700-705.	7.8	23
47	Hydrogen Bonds Control Single-Chain Conformation, Crystallinity, and Electron Transport in Isoelectronic Diketopyrrolopyrrole Copolymers. <i>Chemistry of Materials</i> , 2021, 33, 2635-2645.	6.7	23
48	Adsorption of nucleotides on the rutile (110) surface. <i>International Journal of Materials Research</i> , 2010, 101, 758-764.	0.3	22
49	Defect-induced magnetism in graphite through neutron irradiation. <i>Physical Review B</i> , 2014, 90, .	3.2	21
50	Probing a crystal's short-range structure and local orbitals by Resonant X-ray Diffraction methods. <i>Crystal Research and Technology</i> , 2014, 49, 43-54.	1.3	21
51	Enhancing the magnetic moment of ferrimagnetic NiCo ₂ O ₄ via ion irradiation driven oxygen vacancies. <i>APL Materials</i> , 2018, 6, .	5.1	21
52	Ab initio analysis of electron energy loss spectra for complex oxides. <i>Ultramicroscopy</i> , 1999, 80, 145-151.	1.9	20
53	Surface modeling and chemical solution deposition of SrO(SrTiO ₃) Ruddlesden–Popper phases. <i>Acta Materialia</i> , 2010, 58, 4650-4659.	7.9	20
54	Aging of the (2+1)-dimensional Kardar-Parisi-Zhang model. <i>Physical Review E</i> , 2014, 89, 032146.	2.1	20

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55	Elastic properties and electronic structure of vanadium silicides-a density functional investigation. <i>Acta Materialia</i> , 2009, 57, 50-55.	7.9	19
56	Non-equilibrium dynamics of magnetically anisotropic particles under oscillating fields. <i>European Physical Journal E</i> , 2016, 39, 69.	1.6	19
57	Nickel-enhanced graphitic ordering of carbon ad-atoms during physical vapor deposition. <i>Carbon</i> , 2016, 100, 656-663.	10.3	19
58	Transparent conductive tantalum doped tin oxide as selectively solar-transmitting coating for high temperature solar thermal applications. <i>Solar Energy Materials and Solar Cells</i> , 2019, 196, 84-93.	6.2	19
59	Analysis of the defect clusters in congruent lithium tantalate. <i>Physical Review Materials</i> , 2018, 2, .	2.4	18
60	Li doped MoS ₂ nanowires: elastic and electronic properties. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 3320-3324.	1.5	17
61	Transition metal sulfide clusters below the cluster-platelet transition: Theory and experiment. <i>Physica Status Solidi (B): Basic Research</i> , 2010, 247, 1069-1076.	1.5	17
62	Universality of (2+1)-dimensional restricted solid-on-solid models. <i>Physical Review E</i> , 2016, 94, 022107.	2.1	17
63	Towards Reconfigurable Electronics: Silicidation of Top-Down Fabricated Silicon Nanowires. <i>Applied Sciences (Switzerland)</i> , 2019, 9, 3462.	2.5	16
64	Structure and properties of dimer, trimer and tetramer aggregates of methyltrioxorhenium (MTO): an ab initio study. <i>Journal of Organometallic Chemistry</i> , 1996, 514, 111-117.	1.8	15
65	Electronic structure of Ga ₈₄ cluster compounds. <i>Physical Review B</i> , 2004, 70, .	3.2	15
66	Impurity and vacancy clustering at the $\sqrt{3}(111)[1\bar{1}0]$ grain boundary in strontium titanate. <i>Chemical Physics</i> , 2005, 309, 3-13.	1.9	15
67	Ab-initio calculation of exchange interactions in YMnO ₃ . <i>Computational Materials Science</i> , 2008, 44, 79-81.	3.0	15
68	Molecular dynamics simulations of BMP adsorption on a hydrophobic surface. <i>Materialwissenschaft Und Werkstofftechnik</i> , 2010, 41, 1048-1053.	0.9	15
69	Electron microscopy, spectroscopy, and first-principles calculations of Cs ₂ O. <i>Journal of Solid State Chemistry</i> , 2005, 178, 1190-1196.	2.9	14
70	Feasible Device Architectures for Ultrascaled CNTFETs. <i>IEEE Nanotechnology Magazine</i> , 2018, 17, 100-107.	2.0	14
71	One-dimensional (MoS ₂) _n clusters: Building blocks of clusters materials and ideal nanowires for molecular electronics. <i>Chemical Physics Letters</i> , 2009, 474, 127-131.	2.6	13
72	Tunable discotic building blocks for liquid crystalline displays. <i>Journal of Luminescence</i> , 2004, 108, 143-147.	3.1	12

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73	Compositionally modulated ripples during composite film growth: Three-dimensional pattern formation at the nanoscale. <i>Physical Review B</i> , 2014, 89, .	3.2	12
74	Tetrahedral Amorphous Carbon Coatings for Friction Reduction of the Valve Train in Internal Combustion Engines. <i>Advanced Engineering Materials</i> , 2014, 16, 1226-1233.	3.5	12
75	Structural and electronic properties of Mo ₆ S ₈ clusters deposited on a Au(111) surface investigated with density functional theory. <i>Physical Review B</i> , 2007, 75, .	3.2	11
76	Tilting of carbon encapsulated metallic nanocolumns in carbon-nickel nanocomposite films by ion beam assisted deposition. <i>Applied Physics Letters</i> , 2012, 101, 053112.	3.3	11
77	Hopping-Based Charge Transfer in Diketopyrrolopyrrole-Based Donor-Acceptor Polymers: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2016, 120, 9581-9587.	3.1	11
78	Field-responsive colloidal assemblies defined by magnetic anisotropy. <i>Physical Review E</i> , 2019, 100, 012608.	2.1	11
79	Electron Mobility of Diketopyrrolopyrrole Copolymers Is Robust against Homocoupling Defects. <i>Chemistry of Materials</i> , 2021, 33, 668-677.	6.7	11
80	Observation of Room-Temperature Dark Exciton Emission in Nanopatch-Decorated Monolayer WSe ₂ on Metal Substrate. <i>Advanced Optical Materials</i> , 2021, 9, 2101801.	7.3	11
81	Carbon-nickel nanocomposite templates pre-defined stable catalysts for diameter-controlled growth of single-walled carbon nanotubes. <i>Nanoscale</i> , 2016, 8, 14888-14897.	5.6	10
82	Validity of the dipole-selection rule for the Al-L _{2,3} edge of $\hat{\pm}$ -Al ₂ O ₃ under channeling conditions. <i>Ultramicroscopy</i> , 2001, 88, 253-263.	1.9	9
83	Semi-flexible star-shaped molecules: conformational analysis of nano-segregated mesogens forming columnar liquid-crystal phases. <i>International Journal of Materials Research</i> , 2005, 96, 988-997.	0.8	9
84	Surface-near modifications of SrTiO ₃ local symmetry due to nitrogen implantation investigated by grazing incidence XANES. <i>Scripta Materialia</i> , 2014, 86, 1-4.	5.2	9
85	Thermally induced formation of metastable nanocomposites in amorphous Cr-Zr-O thin films deposited using reactive ion beam sputtering. <i>Thin Solid Films</i> , 2016, 612, 430-436.	1.8	9
86	Dynamical universality classes of simple growth and lattice gas models. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2018, 51, 035003.	2.1	9
87	Success and limits of common final-state approximations. <i>Ultramicroscopy</i> , 2001, 86, 319-324.	1.9	8
88	Evidence for high negative charge densities in AlF ₃ coatings on oxidized silicon: a promising source for large drift fields. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2002, 14, 259-262.	2.7	8
89	Polymorphism in liquid crystals from star-shaped mesogens. <i>Philosophical Magazine Letters</i> , 2007, 87, 883-891.	1.2	8
90	TiSi ₂ nanostructures enhanced conductivity at nanoscale?. <i>Physica Status Solidi (B): Basic Research</i> , 2007, 244, 3593-3600.	1.5	8

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91	Elastic and piezoresistive properties of nickel carbides from first principles. <i>Physical Review B</i> , 2017, 95, .	3.2	8
92	Functional thiols as repair and doping agents of defective MoS ₂ monolayers. <i>Journal of Physics Condensed Matter</i> , 2018, 30, 235302.	1.8	8
93	Tunable Magnetic Vortex Dynamics in Ion-Implanted Permalloy Disks. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 27812-27818.	8.0	8
94	Density-functional study of Mo ₄ S ₆ on Au(111). <i>Applied Physics A: Materials Science and Processing</i> , 2006, 82, 175-179.	2.3	7
95	Microstructural Studies of Fluorine-implanted Titanium Aluminides for Enhanced Environmental Durability. <i>Advanced Engineering Materials</i> , 2014, 16, 52-59.	3.5	7
96	Influence of Electric Fields on the Electron Transport in Donor-Acceptor Polymers. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3714-3723.	3.1	7
97	Electron transport through NiSi ₂ -Si contacts and their role in reconfigurable field-effect transistors. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 355002.	1.8	7
98	Directionality of metal-induced crystallization and layer exchange in amorphous carbon/nickel thin film stacks. <i>Carbon</i> , 2020, 159, 656-667.	10.3	7
99	Formation and crystallographic orientation of NiSi ₂ -Si interfaces. <i>Journal of Applied Physics</i> , 2020, 128, 085301.	2.5	7
100	Modelling ferroic functional elements. <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 211-218.	0.7	6
101	Two-scale modeling of adsorption processes at structured surfaces. <i>Physica D: Nonlinear Phenomena</i> , 2009, 238, 117-125.	2.8	6
102	Environment Controlled Dewetting of Rh-Pd Bilayers: A Route for Core-Shell Nanostructure Synthesis. <i>Journal of Physical Chemistry C</i> , 2012, 116, 14401-14407.	3.1	6
103	Percolated Si:SiO ₂ Nanocomposites: Oven- vs. Millisecond Laser-Induced Crystallization of SiO _x Thin Films. <i>Nanomaterials</i> , 2018, 8, 525.	4.1	6
104	Probing interlayer excitons in a vertical van der Waals p-n junction using a scanning probe microscopy technique. <i>Journal of Physics Condensed Matter</i> , 2019, 31, 114001.	1.8	6
105	Radially resolved electronic structure and charge carrier transport in silicon nanowires. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019, 108, 181-186.	2.7	6
106	Theoretical evidence for the Peierls transition in NbO_2 . <i>Physical Review B</i> , 2021, 104, .	3.2	6
107	Anisotropy of colloidal components propels field-activated stirrers and movers. <i>Physical Review Research</i> , 2020, 2, .	3.6	6
108	Controlling excitons in the quantum tunneling regime in a hybrid plasmonic/2D semiconductor interface. <i>Applied Physics Reviews</i> , 2022, 9, 031401.	11.3	6

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109	Current without external bias and diode effect in shuttling transport of nanoshafts. <i>New Journal of Physics</i> , 2008, 10, 103014.	2.9	5
110	SWCNT growth from C:Ni nanocomposites. <i>Physica Status Solidi (B): Basic Research</i> , 2012, 249, 2357-2360.	1.5	5
111	Theoretical study on the CH ₂ NC hydrogen bond interaction in thiophene-based molecules. <i>Computational and Theoretical Chemistry</i> , 2013, 1005, 45-52.	2.5	5
112	Effects of the TiO ₂ buffer thickness on SrTiO ₃ (111) epitaxial films grown on GaN (0002). <i>Journal of Applied Physics</i> , 2013, 113, 154103.	2.5	5
113	DFT Investigation of the Heterostructure GaP(001) on Si(001). <i>Nanoscience and Nanotechnology Letters</i> , 2013, 5, 73-77.	0.4	5
114	Local scale-invariance of the 2+1 dimensional Kardar-Parisi-Zhang model. <i>Journal of Physics A: Mathematical and Theoretical</i> , 2017, 50, 12LT01.	2.1	5
115	Influence of Nickel Catalyst Morphology on Layer-Exchange-Based Carbon Crystallisation of Ni/a-C Bilayers. <i>Physica Status Solidi (B): Basic Research</i> , 2017, 254, 1700234.	1.5	5
116	Cluster Tool for In Situ Processing and Comprehensive Characterization of Thin Films at High Temperatures. <i>Analytical Chemistry</i> , 2018, 90, 7837-7842.	6.5	5
117	Single-Molecule Doping: Conductance Changed By Transition Metal Centers in Salen Molecules. <i>Advanced Electronic Materials</i> , 2021, 7, 2100252.	5.1	5
118	Autocorrected off-axis holography of two-dimensional materials. <i>Physical Review Research</i> , 2020, 2, .	3.6	5
119	Density-functional investigation of alloyed metallic nanowires. <i>Computer Physics Communications</i> , 2005, 169, 57-59.	7.5	4
120	Tribological Aspects of Carbon-Based Nanocoatings – Theory and Simulation. <i>Zeitschrift Fur Physikalische Chemie</i> , 2011, 225, 379-387.	2.8	4
121	Stoichiometry variation for the atomic layer deposition of Sr _x Ti _y O _z from Sr(iPr ₃ Cp) ₂ , Ti[N(CH ₃) ₂] ₄ and H ₂ O. <i>Thin Solid Films</i> , 2015, 577, 134-142.	1.8	4
122	Suppressing correlations in massively parallel simulations of lattice models. <i>Computer Physics Communications</i> , 2017, 220, 205-211.	7.5	4
123	Tuning the conductance of a molecular wire by the interplay of donor and acceptor units. <i>Nanoscale</i> , 2018, 10, 17131-17139.	5.6	4
124	Formation, structure, and optical properties of copper chromite thin films for high-temperature solar absorbers. <i>Materialia</i> , 2021, 18, 101156.	2.7	4
125	A combined experimental and theoretical study of 1,4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene adsorption on Au(111). <i>Surface Science</i> , 2021, 712, 121877.	1.9	4
126	Oxidative corrosion of adhesive interlayers. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 5140-5144.	2.8	3

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127	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
128	Comparison of atomistic quantum transport and numerical device simulation for carbon nanotube field-effect transistors. , 2016, , .		3
129	Rotational friction of dipolar colloids measured by driven torsional oscillations. Scientific Reports, 2016, 6, 34193.	3.3	3
130	Localization of edge states at triangular defects in periodic MoS_2 monolayers. Physical Review Materials, 2021, 5, .	2.4	3
131	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
132	Low-temperature modeling for degenerate and frustrated Heisenberg systems with anisotropy. Computer Physics Communications, 2010, 181, 806-812.	7.5	2
133	A Two-Parameter Model for Colloidal Particles with an Extended Magnetic Cap. Physica Status Solidi (A) Applications and Materials Science, 2019, 216, 1900506.	1.8	2
134	Interactions of Ruddlesden-Popper Phases and Migration-Induced Field-Stabilized Polar Phase in Strontium Titanate. Crystals, 2021, 11, 693.	2.2	2
135	Theoretical Investigation of Interfaces. Springer Series in Materials Science, 2007, , 91-122.	0.6	2
136	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
137	Binding properties between ferroic oxides and metals. European Physical Journal B, 2009, 67, 57-62.	1.5	1
138	Phase Segregation and Transformations in Arsenic-Implanted ZnO Thin Films. Journal of Physical Chemistry C, 2011, 115, 8798-8807.	3.1	1
139	Band gap tuning of carbon nanotubes for sensor and interconnect applications — A quantum simulation study. , 2012, , .		1
140	Resistive switching in thermally oxidized titanium films. , 2013, , .		1
141	Theoretical investigation of in situ k-restore processes for damaged ultra-low-k materials. , 2015, , .		1
142	Theoretical investigation of in situ k-restore processes for damaged ultra-low-k dielectrics. Microelectronic Engineering, 2016, 156, 121-125.	2.4	1
143	Bit-vectorized GPU implementation of a stochastic cellular automaton model for surface growth. , 2016, , .		1
144	Phase Transitions in C:Ni Nanocomposite Templates during Diameter-Selective CVD Synthesis of SWCNTs. Physica Status Solidi (B): Basic Research, 2017, 254, 1700228.	1.5	1

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145	Direct Correction of Residual Symmetric Aberrations in Electron Holograms of Weak Phase Objects. <i>Microscopy and Microanalysis</i> , 2019, 25, 98-99.	0.4	1
146	Describing chain-like assembly of ethoxygroup-functionalized organic molecules on Au(111) using high-throughput simulations. <i>Scientific Reports</i> , 2021, 11, 14649.	3.3	1
147	Quantum transport and microwave scattering on fractal lattices. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2022, 237, 179-190.	0.8	1
148	Deposition of Nanosized Amino Acid Functionalized Bismuth Oxido Clusters on Gold Surfaces. <i>Nanomaterials</i> , 2022, 12, 1815.	4.1	1
149	Molecular Dynamics. <i>ChemInform</i> , 2004, 35, no.	0.0	0
150	Reduction of surface coverage of finite systems due to geometrical steps. <i>European Physical Journal B</i> , 2008, 62, 311-317.	1.5	0
151	Back Cover: High resolution TEM study of WS ₂ nanotubes (<i>Phys. Status Solidi B</i> 11/2011). <i>Physica Status Solidi (B): Basic Research</i> , 2011, 248, .	1.5	0
152	Closed-Loop Defect States in 2D Materials with Honeycomb Lattice Structure: Molybdenum Disulfide. <i>Physica Status Solidi (B): Basic Research</i> , 2021, 258, 2100214.	1.5	0
153	DFT modelling of defects in strontium titanate. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s208-s209.	0.3	0
154	Reversible structural changes by electrostatic fields in strontium titanate at room temperature. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s232-s232.	0.3	0
155	Correlation of structure and conductance in nanowires. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s155-s155.	0.3	0
156	XRD, XAS and DFT study of the multiferroic mixed-valence compound YMn ₂ O ₅ . <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010, 66, s39-s40.	0.3	0
157	Structure variations within certain rare earth disilicides. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2017, 73, C287-C287.	0.1	0