Gotthard Seifert

List of Publications by Year in descending order

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211 papers	13,955 citations	16411 64 h-index	23472 111 g-index
222 all docs	222 docs citations	222 times ranked	16625 citing authors

#	Article	IF	Citations
1	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, .	0.9	3
2	Closedâ€Loop Defect States in 2D Materials with Honeycomb Lattice Structure: Molybdenum Disulfide. Physica Status Solidi (B): Basic Research, 2021, 258, 2100214.	0.7	0
3	Interfacial Approach toward Benzeneâ€Bridged Polypyrrole Filmâ€"Based Microâ€Supercapacitors with Ultrahigh Volumetric Power Density. Advanced Functional Materials, 2020, 30, 1908243.	7.8	60
4	Exciton <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>g</mml:mi></mml:math> factors of van der Waals heterostructures from first-principles calculations. Physical Review B, 2020, 101, .	1.1	82
5	Unconventional deformation potential and half-metallicity in zigzag nanoribbons of 2D-Xenes. Physical Chemistry Chemical Physics, 2020, 22, 7294-7299.	1.3	4
6	TETT-functionalized TiO2 nanoparticles for DOX loading: a quantum mechanical study at the atomic scale. Nanoscale Advances, 2020, 2, 2774-2784.	2.2	6
7	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	0.7	15
8	Synthetic 2-D lead tin sulfide nanosheets with tuneable optoelectronic properties from a potentially scalable reaction pathway. Chemical Science, 2019, 10, 1035-1045.	3.7	16
9	Twist-driven separation of p-type and n-type dopants in single-crystalline nanowires. National Science Review, 2019, 6, 532-539.	4.6	12
10	Luminescent Emission of Excited Rydberg Excitons from Monolayer WSe₂. Nano Letters, 2019, 19, 2464-2471.	4.5	51
11	An efficient way to model complex magnetite: Assessment of SCC-DFTB against DFT. Journal of Chemical Physics, 2019, 150, 094703.	1.2	24
12	Twist-induced preferential distribution of dopants in single-crystalline Si nanowires. Physical Review B, 2019, 100, .	1.1	6
13	Copolymers of Diketopyrrolopyrrole and Benzothiadiazole: Design and Function from Simulations with Experimental Support. Macromolecules, 2019, 52, 904-914.	2.2	9
14	Surface-Charge Dependent Orientation of Water at the Interface of a Gold Electrode: A Cluster Study. Zeitschrift Fur Physikalische Chemie, 2018, 232, 1583-1592.	1.4	3
15	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	6.5	229
16	A comparative analysis of symmetric diketopyrrolopyrroleâ€cored small conjugated molecules with aromatic flanks: From geometry to charge transport. Journal of Computational Chemistry, 2018, 39, 2526-2538.	1.5	7
17	Theoretical and experimental investigations of ¹²⁹Xe NMR chemical shift isotherms in metalâ€"organic frameworks. Physical Chemistry Chemical Physics, 2018, 20, 25039-25043.	1.3	8
18	Functional thiols as repair and doping agents of defective MoS₂ monolayers. Journal of Physics Condensed Matter, 2018, 30, 235302.	0.7	8

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19	Curved TiO₂ Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. ACS Applied Materials & Interfaces, 2018, 10, 29943-29953.	4.0	35
20	Graphite oxide swelling in molten sugar alcohols and their aqueous solutions. Carbon, 2018, 140, 157-163.	5.4	15
21	Molecular Doping of a High Mobility Diketopyrrolopyrroleâ€“Dithienylthieno[3,2-b]thiophene Donorâ€“Acceptor Copolymer with F6TCNNQ. Macromolecules, 2017, 50, 914-926.	2.2	66
22	Localized defect states in MoS₂monolayers: Electronic and optical properties. Physica Status Solidi (B): Basic Research, 2017, 254, 1600645.	0.7	30
23	Charge Transfer Variability in Misfit Layer Compounds: Comparison of SnSâ€“SnS₂ and LaSâ€“TaS₂. Israel Journal of Chemistry, 2017, 57, 553-559.	1.0	10
24	Influence of Electric Fields on the Electron Transport in Donorâ€“Acceptor Polymers. Journal of Physical Chemistry C, 2017, 121, 3714-3723.	1.5	7
25	Porous graphite oxide pillared with tetrapod-shaped molecules. Carbon, 2017, 120, 145-156.	5.4	29
26	Multilayered intercalation of 1-octanol into Brodie graphite oxide. Nanoscale, 2017, 9, 6929-6936.	2.8	27
27	Tuning quantum electron and phonon transport in two-dimensional materials by strain engineering: a Green's function based study. Physical Chemistry Chemical Physics, 2017, 19, 1487-1495.	1.3	19
28	The origin of the measured chemical shift of ¹²⁹Xe in UiO-66 and UiO-67 revealed by DFT investigations. Physical Chemistry Chemical Physics, 2017, 19, 10020-10027.	1.3	23
29	Molybdenum Carbide-Embedded Nitrogen-Doped Porous Carbon Nanosheets as Electrocatalysts for Water Splitting in Alkaline Media. ACS Nano, 2017, 11, 3933-3942.	7.3	367
30	Structure and Stability of GaS Fullerenes and Nanotubes. Israel Journal of Chemistry, 2017, 57, 529-539.	1.0	6
31	Chemical and Electronic Repair Mechanism of Defects in MoS₂ Monolayers. ACS Nano, 2017, 11, 9989-9996.	7.3	80
32	Toward Activity Origin of Electrocatalytic Hydrogen Evolution Reaction on Carbonâ€Rich Crystalline Coordination Polymers. Small, 2017, 13, 1700783.	5.2	16
33	Effective Zeeman splitting in bent lateral heterojunctions of graphene and hexagonal boron nitride: A new mechanism towards half-metallicity. Physical Review B, 2017, 96, .	1.1	14
34	Water Multilayers on TiO₂ (101) Anatase Surface: Assessment of a DFTB-Based Method. Journal of Chemical Theory and Computation, 2017, 13, 3862-3873.	2.3	40
35	Conformational and electronic properties of small benzothiadiazole-cored oligomers with aryl flanking units: Thiophene versus Furan. Computational Materials Science, 2017, 126, 287-298.	1.4	21
36	Immobilizing Molecular Metal Dithioleneâ€“Diamine Complexes on 2D Metalâ€“Organic Frameworks for Electrocatalytic H₂ Production. Chemistry - A European Journal, 2017, 23, 2255-2260.	1.7	208

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37	Impact of incomplete metal coverage on the electrical properties of metal-CNT contacts: A large-scale ab initio study. Applied Physics Letters, 2016, 109, .	1.5	10
38	Towards an optimal contact metal for CNTFETs. Nanoscale, 2016, 8, 10240-10251.	2.8	54
39	Hopping-Based Charge Transfer in Diketopyrrolopyrrole-Based Donorâ€“Acceptor Polymers: A Theoretical Study. Journal of Physical Chemistry C, 2016, 120, 9581-9587.	1.5	11
40	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
41	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.	11.1	130
42	Screening for high-spin metal organic frameworks (MOFs): density functional theory study on DUT-8(M₁,M₂) (with M_i = V,â€¦,Cu). Physical Chemistry Chemical Physics, 2016, 18, 8075-8080.	1.3	23
43	Tubular structures from the LnSâ€“TaS₂ (Ln = La, Ce, Nd, Ho, Er) and LaSeâ€“TaSe₂ misfit layered compounds. Journal of Materials Chemistry C, 2016, 4, 89-98.	2.7	22
44	Electronic and magnetic properties of DUT-8(Ni). Physical Chemistry Chemical Physics, 2015, 17, 17122-17129.	1.3	29
45	Hydrogen adsorption by perforated graphene. International Journal of Hydrogen Energy, 2015, 40, 6594-6599.	3.8	59
46	Enhanced proton-transfer activity in imidazole@MIL-53(Al) systems revealed by molecular-dynamics simulations. Microporous and Mesoporous Materials, 2015, 216, 36-41.	2.2	12
47	Characteristics of flexibility in metal-organic framework solid solutions of composition [Zn2(BME-bdc)x(DB-bdc)2â^'xdabco]n: In situ powder X-ray diffraction, in situ NMR spectroscopy, and molecular dynamics simulations. Microporous and Mesoporous Materials, 2015, 216, 64-74.	2.2	41
48	Graphene-based technologies for energy applications, challenges and perspectives. 2D Materials, 2015, 2, 030204.	2.0	74
49	Nanotube Electromechanics beyond Carbon: The Case of WS₂. ACS Nano, 2015, 9, 12224-12232.	7.3	29
50	Hydrogen storage in high surface area graphene scaffolds. Chemical Communications, 2015, 51, 15280-15283.	2.2	79
51	Tin(II) Sulfide (SnS) Nanosheets by Liquid-Phase Exfoliation of Herzenbergite: IVâ€“VI Main Group Two-Dimensional Atomic Crystals. Journal of the American Chemical Society, 2015, 137, 12689-12696.	6.6	220
52	Porous Graphene Oxide/Diboronic Acid Materials: Structure and Hydrogen Sorption. Journal of Physical Chemistry C, 2015, 119, 27179-27191.	1.5	49
53	Optics, Mechanics, and Energetics of Two-Dimensional MoS₂ Nanostructures from a Theoretical Perspective. Accounts of Chemical Research, 2015, 48, 48-55.	7.6	53
54	Single- to Triple-Wall WS2 Nanotubes Obtained by High-Power Plasma Ablation of WS2 Multiwall Nanotubes. Inorganics, 2014, 2, 177-190.	1.2	27

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55	Two-dimensional and tubular structures of misfit compounds: Structural and electronic properties. Beilstein Journal of Nanotechnology, 2014, 5, 2171-2178.	1.5	14
56	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. Tribology Letters, 2014, 53, 119-126.	1.2	89
57	Density functional tight binding. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120483.	1.6	256
58	Optical Properties of Triangular Molybdenum Disulfide Nanoflakes. Journal of Physical Chemistry Letters, 2014, 5, 3636-3640.	2.1	35
59	Is MoS2a robust material for 2D electronics?. Nanotechnology, 2014, 25, 445201.	1.3	14
60	Tetrahedral Amorphous Carbon Coatings for Friction Reduction of the Valve Train in Internal Combustion Engines. Advanced Engineering Materials, 2014, 16, 1226-1233.	1.6	12
61	Proton Conduction in a MIL-53(Al) Metalâ€“Organic Framework: Confinement versus Host/Guest Interaction. Journal of Physical Chemistry C, 2014, 118, 13035-13041.	1.5	35
62	Combined SnS@SnS₂double layers: charge transfer and electronic structure. Semiconductor Science and Technology, 2014, 29, 064006.	1.0	23
63	Stretching and breaking of monolayer MoS ₂ â€”an atomistic simulation. 2D Materials, 2014, 1, 011007.	2.0	32
64	Dielectric Properties of Selected Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 11799-11805.	1.5	40
65	Gate effects in a hexagonal zinc-imidazolate-4-amide-5-imidate framework with flexible methoxy substituents and CO2 selectivity. Chemical Communications, 2013, 49, 7599.	2.2	35
66	Syntheses of two imidazolate-4-amide-5-imidate linker-based hexagonal metalâ€“organic frameworks with flexible ethoxy substituent. CrystEngComm, 2013, 15, 9394.	1.3	27
67	The Virtues of Magnetism. ACS Nano, 2013, 7, 10449-10451.	7.3	6
68	Quantifying charge transfer energies at donorâ€“acceptor interfaces in small-molecule solar cells with constrained DFTB and spectroscopic methods. Journal of Physics Condensed Matter, 2013, 25, 473201.	0.7	38
69	Theoretical studies on the structural and electronic properties of Ï€-stacked cyano-thiophene-based molecules. Computational and Theoretical Chemistry, 2013, 1023, 65-73.	1.1	4
70	Theoretical study on the CHâ‹¯NC hydrogen bond interaction in thiophene-based molecules. Computational and Theoretical Chemistry, 2013, 1005, 45-52.	1.1	5
71	Observation of a Bursteinâ€“Moss Shift in Rhenium-Doped MoS₂ Nanoparticles. ACS Nano, 2013, 7, 3506-3511.	7.3	81
72	Line Defects in Molybdenum Disulfide Layers. Journal of Physical Chemistry C, 2013, 117, 10842-10848.	1.5	127

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73	Defect-induced conductivity anisotropy in MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>monolayers. Physical Review B, 2013, 88, .	1.1	144
74	Theoretical investigation of the electronic structure and quantum transport in the grapheneâ€“C(111) diamond surface system. Journal of Physics Condensed Matter, 2013, 25, 435302.	0.7	13
75	Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. Physical Review B, 2013, 88, .	1.1	16
76	Optimizing Electronic Structure and Quantum Transport at the Graphene-Si(111) Interface: AnAbÂInitioDensity-Functional Study. Physical Review Letters, 2013, 110, 176805.	2.9	23
77	Squeezing lone pairs: The<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi></mml:math>17 to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>A</mml:mi></mml:math>7 pressure-induced phase transition in black phosphorus. Physical Review B, 2013, 87, .	1.1	81
78	Nanomechanical Energy Storage in Twisted Nanotube Ropes. Physical Review Letters, 2012, 109, 255501.	2.9	18
79	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Physikalische Chemie, 2012, 226, 95-106.	1.4	4
80	Combined IR absorption and modeling study of nanoporous zeolite imidazolate frameworks (ZIFs) filled with hydrogen. RSC Advances, 2012, 2, 9839.	1.7	4
81	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1555-1555.	0.6	0
82	Designing Electrical Contacts to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Monolayers: A Computational Study. Physical Review Letters, 2012, 108, 156802.	7.9	475
83	Density-functional study of LixMoS2 intercalates (0â©½xâ©½1). Computational and Theoretical Chemistry, 2012, 999, 13-20.	1.1	120
84	Structural properties of metalâ€organic frameworks within the densityâ€functional based tightâ€binding method. Physica Status Solidi (B): Basic Research, 2012, 249, 335-342.	0.7	42
85	Densityâ€functional tight bindingâ€”an approximate densityâ€functional theory method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 456-465.	6.2	175
86	Helicity in Ropes of Chiral Nanotubes: Calculations and Observation. Physical Review Letters, 2012, 108, 235501.	2.9	6
87	Theoretical Study of the Mechanical Behavior of Individual TiS₂ and MoS₂ Nanotubes. Journal of Physical Chemistry C, 2012, 116, 11714-11721.	1.5	114
88	An Isoreticular Family of Microporous Metalâ€“Organic Frameworks Based on Zinc and 2â€Substituted Imidazolateâ€4â€amideâ€5â€imidate: Syntheses, Structures and Properties. Chemistry - A European Journal, 2012, 18, 11630-11640.	1.7	26
89	Controlled Doping of MS₂ (M=W, Mo) Nanotubes and Fullereneâ€like Nanoparticles. Angewandte Chemie - International Edition, 2012, 51, 1148-1151.	7.2	73
90	Polymorphs of lithium-boron imidazolates: energy landscape and hydrogen storage properties. Dalton Transactions, 2011, 40, 3796-3798.	1.6	22

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91	Structural and Electronic Properties of Helical TiS₂ Nanotubes Studied with Objective Molecular Dynamics. Journal of Physical Chemistry C, 2011, 115, 6392-6396.	1.5	27
92	High-Pressure in Situ ¹²⁹Xe NMR Spectroscopy and Computer Simulations of Breathing Transitions in the Metalâ€“Organic Framework Ni₂(2,6-ndc)₂(dabco) (DUT-8(Ni)). Journal of the American Chemical Society, 2011, 133, 8681-8690.	6.6	113
93	New Route for Stabilization of 1T-WS₂ and MoS₂ Phases. Journal of Physical Chemistry C, 2011, 115, 24586-24591.	1.5	430
94	Optical Excitations in CdSe/CdS Coreâ€“Shell Nanoparticles. Journal of Physical Chemistry C, 2011, 115, 10338-10344.	1.5	7
95	Experimental, finite element, and density-functional theory study of inorganic nanotube compression. Applied Physics Letters, 2011, 98, 081908.	1.5	14
96	High resolution TEM study of WS₂ nanotubes. Physica Status Solidi (B): Basic Research, 2011, 248, 2716-2719.	0.7	35
97	Packings of Carbon Nanotubes â€“ New Materials for Hydrogen Storage. Advanced Materials, 2011, 23, 1237-1241.	11.1	76
98	MoS₂ Hybrid Nanostructures: From Octahedral to Quasiâ€Spherical Shells within Individual Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 1810-1814.	7.2	62
99	Synthesis of Copious Amounts of SnS₂ and SnS₂/SnS Nanotubes with Ordered Superstructures. Angewandte Chemie - International Edition, 2011, 50, 12316-12320.	7.2	94
100	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. International Journal of Hydrogen Energy, 2011, 36, 6005-6013.	3.8	38
101	Radial compression studies of WS2 nanotubes in the elastic regime. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2011, 29, .	0.6	18
102	Novel Computational Approaches to Li Diffusion and Electron Transport for High Capacity Battery Materials. Materials Research Society Symposia Proceedings, 2011, 1313, 70101.	0.1	0
103	Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. Journal of Physical Chemistry C, 2010, 114, 11358-11363.	1.5	231
104	Molecular-dynamics simulations of capillary imbibition of KI melt into MoS2 nanotubes. Chemical Physics Letters, 2010, 501, 98-102.	1.2	5
105	Oneâ€and Twoâ€Dimensional Inorganic Crystals inside Inorganic Nanotubes. European Journal of Inorganic Chemistry, 2010, 2010, 4233-4243.	1.0	14
106	Synthesis of Coreâ€“Shell Inorganic Nanotubes. Advanced Functional Materials, 2010, 20, 2459-2468.	7.8	54
107	Adsorption of hydrogen in covalent organic frameworks: Comparison of simulations and experiments. Microporous and Mesoporous Materials, 2010, 133, 59-65.	2.2	58
108	Hydrogen adsorption sites and energies in 2D and 3D covalent organic frameworks. Chemical Physics Letters, 2010, 489, 86-91.	1.2	27

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109	Selfâ€assembled Monolayers of Alkylphosphonic Acids on Aluminum Oxide Surfaces â€“ A Theoretical Study. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 1506-1512.	0.6	38
110	Transition metal sulfide clusters below the clusterâ€“platelet transition: Theory and experiment. Physica Status Solidi (B): Basic Research, 2010, 247, 1069-1076.	0.7	17
111	Prediction of huge magnetic anisotropies of transition-metal dimer-benzene complexes from density functional theory calculations. Physical Review B, 2010, 82, .	1.1	18
112	Hydrogen Adsorption Sites in Zeolite Imidazolate Frameworks ZIF-8 and ZIF-11. Journal of Physical Chemistry C, 2010, 114, 13381-13384.	1.5	66
113	Adsorption of nucleotides on the rutile (110) surface. International Journal of Materials Research, 2010, 101, 758-764.	0.1	22
114	Hollow V₂O₅ Nanoparticles (Fullerene-Like Analogues) Prepared by Laser Ablation. Journal of the American Chemical Society, 2010, 132, 11214-11222.	6.6	45
115	Stability and Electronic Properties of Bismuth Nanotubes. Journal of Physical Chemistry C, 2010, 114, 22092-22097.	1.5	31
116	Density-functional based tight-binding: an approximate DFT method. Journal of the Brazilian Chemical Society, 2009, 20, 1193-1205.	0.6	177
117	Stability and electronic properties of rhenium sulfide nanotubes. Physica Status Solidi (B): Basic Research, 2009, 246, 114-118.	0.7	8
118	Aspects of the Proton Transfer in Liquid Phosphonic Acid. Journal of Physical Chemistry B, 2009, 113, 8475-8480.	1.2	15
119	Nanoseashells and Nanooctahedra of MoS2: Routes to Inorganic Fullerenes. Chemistry of Materials, 2009, 21, 5627-5636.	3.2	29
120	Capillary Imbibition of PbI₂ Melt by Inorganic and Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 13664-13669.	1.5	26
121	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	1.1	88
122	Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: Application to polycyclic aromatic hydrocarbon clusters. Journal of Chemical Physics, 2009, 130, 244304.	1.2	88
123	Co Dimers on Hexagonal Carbon Rings Proposed as Subnanometer Magnetic Storage Bits. Physical Review Letters, 2009, 103, 187201.	2.9	91
124	Hydrogen storage in 1D nanotube-like channels metalâ€“organic frameworks: Effects of free volume and heat of adsorption on hydrogen uptake. International Journal of Hydrogen Energy, 2009, 34, 8135-8143.	3.8	23
125	Adsorption of Phosphonic Acid at the TiO₂ Anatase (101) and Rutile (110) Surfaces. Journal of Physical Chemistry C, 2009, 113, 5730-5740.	1.5	155
126	On the nature of the interaction between H2 and metal-organic frameworks. Theoretical Chemistry Accounts, 2008, 120, 543-550.	0.5	36

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127	H₂ Adsorption in Metalâ€Organic Frameworks: Dispersion or Electrostatic Interactions?. Chemistry - A European Journal, 2008, 14, 6597-6600.	1.7	69
128	Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. Surface Science, 2008, 602, 1347-1359.	0.8	97
129	Fullereneâ€like Mo(W)_{1â^'x}Re_xS₂ Nanoparticles. Chemistry - an Asian Journal, 2008, 3, 1568-1574.	1.7	33
130	Torsional Stick-Slip Behavior in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Nanotubes. Physical Review Letters, 2008, 101, 195501.	2.9	68
131	Electronic and transport properties of contacts between molybdenum sulfide nanowires and gold electrodes. Applied Physics Letters, 2008, 93, .	1.5	11
132	Nanolubrication: How Do MoS2-Based Nanostructures Lubricate?. Journal of Physical Chemistry C, 2008, 112, 17764-17767.	1.5	64
133	Atom by atom: HRTEM insights into inorganic nanotubes and fullerene-like structures. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 15643-15648.	3.3	77
134	Toward Atomic-Scale Bright-Field Electron Tomography for the Study of Fullerene-Like Nanostructures. Nano Letters, 2008, 8, 891-896.	4.5	61
135	Atomic-Scale Structure of Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 3928-3931.	4.5	68
136	Electromechanical Switch Based on Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 4093-4097.	4.5	45
137	Structural and electronic properties ofMo6S8clusters deposited on a Au(111) surface investigated with density functional theory. Physical Review B, 2007, 75, .	1.1	11
138	Unique Structural and Transport Properties of Molybdenum Chalcohalide Nanowires. Physical Review Letters, 2007, 99, 085503.	2.9	30
139	Treatment of Collinear and Noncollinear Electron Spin within an Approximate Density Functional Based Methodâ€. Journal of Physical Chemistry A, 2007, 111, 5622-5629.	1.1	55
140	Infrared Spectra of Alkylphosphonic Acid Bound to Aluminium Surfaces. Macromolecular Symposia, 2007, 254, 248-253.	0.4	74
141	Titanium oxide fullerenes: electronic structure and basic trends in their stability. Physical Chemistry Chemical Physics, 2007, 9, 5772.	1.3	7
142	Optical Excitations in Cadmium Sulfide Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 10761-10770.	1.5	57
143	Hydrogen Sieving and Storage in Fullerene Intercalated Graphite. Nano Letters, 2007, 7, 1-5.	4.5	92
144	Microscopic Investigation of Shear in Multiwalled Nanotube Deformation. Journal of Physical Chemistry C, 2007, 111, 8432-8436.	1.5	33

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145	Car-Parrinello treatment for an approximate density-functional theory method. Journal of Chemical Physics, 2007, 126, 124103.	1.2	19
146	3dmetal nanowires and clusters inside carbon nanotubes: Structural, electronic, and magnetic properties. Physical Review B, 2007, 75, .	1.1	102
147	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	7.3	172
148	Electronic properties and optical spectra of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Mo</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">W</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>2	1.1	68
149	Structure and Stability of Molybdenum Sulfide Fullerenes. Angewandte Chemie - International Edition, 2007, 46, 623-627.	7.2	84
150	Properties of the phosphonic-acid molecule and the proton transfer in the phosphonic-acid dimer. Computational and Theoretical Chemistry, 2007, 816, 119-123.	1.5	27
151	Curvature effects of nitrogen on graphitic sheets: Structures and energetics. Chemical Physics Letters, 2007, 447, 115-120.	1.2	32
152	Formation, Structure, and Polymorphism of Novel Lowestâ€Dimensional AgI Nanoaggregates by Encapsulation in Carbon Nanotubes. Small, 2007, 3, 1730-1734.	5.2	21
153	Catalysts on the edge. Nature Nanotechnology, 2007, 2, 21-22.	15.6	23
154	Simulation of Inorganic Nanotubes. Springer Series in Materials Science, 2007, , 33-57.	0.4	26
155	Extending the scope of â€˜in silico experimentsâ€™: Theoretical approaches for the investigation of reaction mechanisms, nucleation events and phase transitions. Science and Technology of Advanced Materials, 2007, 8, 434-441.	2.8	10
156	Infrared Spectra of Alkylphosphonic Acid Bound to Aluminium Surfaces. Macromolecular Symposia, 2007, 254, 248-253.	0.4	2
157	On the mechanical behavior of WS2 nanotubes under axial tension and compression. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 523-528.	3.3	263
158	Hexagon-preserving carbon foams: Properties of hypothetical carbon allotropes. Physical Review B, 2006, 74, .	1.1	92
159	MonS2n+x clustersâ€”magic numbers and platelets. Computational Materials Science, 2006, 35, 316-320.	1.4	29
160	Magnetism and the potential energy hypersurfaces of Fe53 to Fe57. Computational Materials Science, 2006, 35, 297-301.	1.4	15
161	Physisorption of N2 on graphene platelets: An Ab initio study. International Journal of Quantum Chemistry, 2006, 106, 1375-1382.	1.0	22
162	Molecular design of fullerene-based ultralow-kdielectrics. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 3868-3872.	0.8	16

#	Article	IF	Citations
163	Theoretical study of the propagation barrier of ethylene polymerization with TiR2 (R=OCH3 or CN): The importance of the Î²-agostic interactions. Computational and Theoretical Chemistry, 2006, 762, 9-15.	1.5	5
164	C28fulleritesâ€"structure, electronic properties and intercalates. Physical Chemistry Chemical Physics, 2006, 8, 3320-3325.	1.3	31
165	Stability and electronic properties of single-walled Î³-AlO(OH) nanotubes. Mendeleev Communications, 2006, 16, 292-294.	0.6	9
166	The Magnetic Shielding Function of Molecules and Pi-Electron Delocalization. ChemInform, 2006, 37, no.	0.1	0
167	Fibrous Red Phosphorus.. ChemInform, 2006, 37, no.	0.1	0
168	Density functional based calculations for Fen (nâ©½32). Chemical Physics, 2005, 309, 23-31.	0.9	146
169	A theoretical study of the structural and electronic properties of CdSe/CdS and CdS/CdSe core/shell nanoparticles. Chemical Physics Letters, 2005, 405, 103-107.	1.2	34
170	From The Cover: Graphene nanostructures as tunable storage media for molecular hydrogen. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10439-10444.	3.3	573
171	The Effects of Organisation, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. European Journal of Inorganic Chemistry, 2005, 2005, 3585-3596.	1.0	33
172	Fibrous Red Phosphorus. Angewandte Chemie - International Edition, 2005, 44, 7616-7619.	7.2	209
173	The Effects of Organization, Embedding and Surfactants on the Properties of Cadmium Chalcogenide (CdS, CdSe and CdS/CdSe) Semiconductor Nanoparticles. ChemInform, 2005, 36, no.	0.1	0
174	DFT Ã—TB â^' a unified quantum-mechanical hybrid method. Theoretical Chemistry Accounts, 2005, 114, 68-75.	0.5	5
175	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	0.6	63
176	Structure, stability and electronic properties of TiO2 nanostructures. Physica Status Solidi (B): Basic Research, 2005, 242, 1361-1370.	0.7	120
177	Molecular Dynamics Study of the Mechanical and Electronic Properties of Carbon Nanotubes. Small, 2005, 1, 399-402.	5.2	16
178	Density-functional-based molecular-dynamics simulations of molten salts. Journal of Chemical Physics, 2005, 123, 134510.	1.2	23
179	Hyperdiamond and hyperlonsdaleit: Possible crystalline phases of fullereneC28. Physical Review B, 2005, 72, .	1.1	31
180	The Magnetic Shielding Function of Molecules and Pi-Electron Delocalization. Chemical Reviews, 2005, 105, 3889-3910.	23.0	182

#	Article	IF	Citations
181	An Efficienta PosterioriTreatment for Dispersion Interaction in Density-Functional-Based Tight Binding. Journal of Chemical Theory and Computation, 2005, 1, 841-847.	2.3	275
182	Planar Tetracoordinate Carbons in Cyclic Hydrocarbons. Organic Letters, 2005, 7, 1509-1512.	2.4	68
183	Induced Magnetic Fields in Aromatic [n]-Annulenes â€" Interpretation of NICS Tensor Components. ChemInform, 2004, 35, no.	0.1	0
184	Hydrogen Storage by Physisorption on Nanostructured Graphite Platelets.. ChemInform, 2004, 35, no.	0.1	1
185	The Induced Magnetic Field in Cyclic Molecules. Chemistry - A European Journal, 2004, 10, 4367-4371.	1.7	266
186	Atomistic Simulation Study of the Pressure Induced Incorporation of Helium into C60. Journal of Physical Chemistry B, 2004, 108, 16495-16498.	1.2	10
187	Semiempirical Methods for the Calculation of NMR Chemical Shifts. , 2004, , 141-152.		2
188	D5h C50 Fullerene:â€‰ A Building Block for Oligomers and Solids?. Journal of Physical Chemistry A, 2004, 108, 11733-11739.	1.1	42
189	Hydrogen storage by physisorption on nanostructured graphite plateletsElectronic supplementary information (ESI) available: Fig. 1S: Potential energy surface of H2 parallel to benzene at the MP2 level. See http://www.rsc.org/suppdata/cp/b3/b316209e/. Physical Chemistry Chemical Physics, 2004, 6, 980.	1.3	168
190	Induced magnetic fields in aromatic [n]-annulenesâ€"interpretation of NICS tensor components. Physical Chemistry Chemical Physics, 2004, 6, 273-276.	1.3	425
191	Optical Properties of Cadmium Sulfide Clusters.. ChemInform, 2003, 34, no.	0.1	0
192	Optical Properties of Cadmium Sulfide Clusters. Journal of Physical Chemistry B, 2003, 107, 2897-2902.	1.2	46
193	Analysis of Aromatic Delocalization:Â Individual Molecular Orbital Contributions to Nucleus-Independent Chemical Shifts. Journal of Physical Chemistry A, 2003, 107, 6470-6475.	1.1	151
194	SiO2-coated carbon nanotubes: theory and experiment. International Journal of Materials Research, 2002, 93, 455-458.	0.8	6
195	Atomistic simulations of complex materials: ground-state and excited-state properties. Journal of Physics Condensed Matter, 2002, 14, 3015-3047.	0.7	423
196	Theoretical tools for transport in molecular nanostructures. Physica B: Condensed Matter, 2002, 314, 86-90.	1.3	75
197	Molecular Devices Simulations Based on Density Functional Tight-Binding. Journal of Computational Electronics, 2002, 1, 109-112.	1.3	8
198	A Hydrogen Storage Mechanism in Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2001, 123, 5059-5063.	6.6	227

#	Article	IF	Citations
199	Tubular structures of germanium. Solid State Communications, 2001, 119, 653-657.	0.9	23
200	Towards controlled production of specific carbon nanostructuresâ€" a theoretical study on structural transformations of graphitic and diamond particles. Applied Physics Letters, 2001, 79, 63-65.	1.5	26
201	On the electronic structure of WS2 nanotubes. Solid State Communications, 2000, 114, 245-248.	0.9	120
202	On the electronic structure of non carbon nanotubes. AIP Conference Proceedings, 2000, , .	0.3	4
203	Molecular wires, solenoids, and capacitors by sidewall functionalization of carbon nanotubes. Applied Physics Letters, 2000, 77, 1313-1315.	1.5	86
204	Ionization Energy of Fullerenes. Journal of the American Chemical Society, 2000, 122, 9745-9749.	6.6	101
205	Structure and Electronic Properties ofMoS2Nanotubes. Physical Review Letters, 2000, 85, 146-149.	2.9	497
206	Structural and Electronic Properties of Cadmium Sulfide Clusters. Journal of Physical Chemistry B, 2000, 104, 2617-2622.	1.2	99
207	Structural and energetic parallels between hydrogenated and fluorinated fullerenes: C36X6. Journal of the Chemical Society Perkin Transactions II, 1999, , 707-712.	0.9	22
208	Concentric-shell fullerenes and diamond particles: A molecular-dynamics study. Physical Review B, 1999, 60, 10711-10714.	1.1	64
209	Vibrational signatures of fullerene oxides. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2287-2294.	1.7	36
210	Collision Energy Dependence of Molecular Fusion and Fragmentation inC60++C60Collisions. Physical Review Letters, 1996, 76, 3289-3292.	2.9	55
211	Eine approximative Variante zur Berechnung der kernmagnetischen Abschirmung von MolekÃ¼len mit Hilfe des UCPâ€X_{Î±}â€Verfahrens. Zeitschrift FÃ¼r Chemie, 1988, 28, 156-157.	0.0	1