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	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
2	Structure and Electronic Properties ofMoS2Nanotubes. Physical Review Letters, 2000, 85, 146-149.	2.9	497
3	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.	2.9	475
4	New Route for Stabilization of 1T-WS₂ and MoS₂ Phases. Journal of Physical Chemistry C, 2011, 115, 24586-24591.	1.5	430
5	Induced magnetic fields in aromatic [n]-annulenesâ€"interpretation of NICS tensor components. Physical Chemistry Chemical Physics, 2004, 6, 273-276.	1.3	425
6	Atomistic simulations of complex materials: ground-state and excited-state properties. Journal of Physics Condensed Matter, 2002, 14, 3015-3047.	0.7	423
7	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
8	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
9	The Induced Magnetic Field in Cyclic Molecules. Chemistry - A European Journal, 2004, 10, 4367-4371.	1.7	266
10	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
11	Density functional tight binding. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20120483.	1.6	256
12	Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. Journal of Physical Chemistry C, 2010, 114, 11358-11363.	1.5	231
13	Momentum-space indirect interlayer excitons in transition-metal dichalcogenide van der Waals heterostructures. Nature Physics, 2018, 14, 801-805.	6.5	229
14	A Hydrogen Storage Mechanism in Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2001, 123, 5059-5063.	6.6	227
15	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
16	Fibrous Red Phosphorus. Angewandte Chemie - International Edition, 2005, 44, 7616-7619.	7.2	209
17	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
18	The Magnetic Shielding Function of Molecules and Pi-Electron Delocalization. Chemical Reviews, 2005, 105, 3889-3910.	23.0	182

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19	Density-functional based tight-binding: an approximate DFT method. Journal of the Brazilian Chemical Society, 2009, 20, 1193-1205.	0.6	177
20	Densityâ€functional tight bindingâ€”an approximate densityâ€functional theory method. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 456-465.	6.2	175
21	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	7.3	172
22	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
23	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
24	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
25	Density functional based calculations for Fen (nâ©½32). Chemical Physics, 2005, 309, 23-31.	0.9	146
26	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
27	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
28	Line Defects in Molybdenum Disulfide Layers. Journal of Physical Chemistry C, 2013, 117, 10842-10848.	1.5	127
29	On the electronic structure of WS2 nanotubes. Solid State Communications, 2000, 114, 245-248.	0.9	120
30	Structure, stability and electronic properties of TiO2 nanostructures. Physica Status Solidi (B): Basic Research, 2005, 242, 1361-1370.	0.7	120
31	Density-functional study of LixMoS2 intercalates (0â©½xâ©½1). Computational and Theoretical Chemistry, 2012, 999, 13-20.	1.1	120
32	Theoretical Study of the Mechanical Behavior of Individual TiS₂ and MoS₂ Nanotubes. Journal of Physical Chemistry C, 2012, 116, 11714-11721.	1.5	114
33	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
34	3dmetal nanowires and clusters inside carbon nanotubes: Structural, electronic, and magnetic properties. Physical Review B, 2007, 75, .	1.1	102
35	Ionization Energy of Fullerenes. Journal of the American Chemical Society, 2000, 122, 9745-9749.	6.6	101
36	Structural and Electronic Properties of Cadmium Sulfide Clusters. Journal of Physical Chemistry B, 2000, 104, 2617-2622.	1.2	99

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37	Adsorption of phosphonic and ethylphosphonic acid on aluminum oxide surfaces. Surface Science, 2008, 602, 1347-1359.	0.8	97
38	Synthesis of Copious Amounts of SnS₂ and SnS₂/SnS Nanotubes with Ordered Superstructures. Angewandte Chemie - International Edition, 2011, 50, 12316-12320.	7.2	94
39	Hexagon-preserving carbon foams: Properties of hypothetical carbon allotropes. Physical Review B, 2006, 74, .	1.1	92
40	Hydrogen Sieving and Storage in Fullerene Intercalated Graphite. Nano Letters, 2007, 7, 1-5.	4.5	92
41	Co Dimers on Hexagonal Carbon Rings Proposed as Subnanometer Magnetic Storage Bits. Physical Review Letters, 2009, 103, 187201.	2.9	91
42	Wear, Plasticity, and Rehybridization in Tetrahedral Amorphous Carbon. Tribology Letters, 2014, 53, 119-126.	1.2	89
43	Nonadiabatic Dynamics within Time-Dependent Density Functional Tight Binding Method. Journal of Physical Chemistry A, 2009, 113, 12700-12705.	1.1	88
44	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
45	Molecular wires, solenoids, and capacitors by sidewall functionalization of carbon nanotubes. Applied Physics Letters, 2000, 77, 1313-1315.	1.5	86
46	Structure and Stability of Molybdenum Sulfide Fullerenes. Angewandte Chemie - International Edition, 2007, 46, 623-627.	7.2	84
47	Anisotropic Thermoelectric Response in Two-Dimensional Puckered Structures. Journal of Physical Chemistry C, 2016, 120, 18841-18849.	1.5	84
48	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
49	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, 2012, 85, .	1.1	81
50	Observation of a Bursteinâ€“Moss Shift in Rhenium-Doped MoS₂ Nanoparticles. ACS Nano, 2013, 7, 3506-3511.	7.3	81
51	Chemical and Electronic Repair Mechanism of Defects in MoS₂ Monolayers. ACS Nano, 2017, 11, 9989-9996.	7.3	80
52	Hydrogen storage in high surface area graphene scaffolds. Chemical Communications, 2015, 51, 15280-15283.	2.2	79
53	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
54	Packings of Carbon Nanotubes â€“ New Materials for Hydrogen Storage. Advanced Materials, 2011, 23, 1237-1241.	11.1	76

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55	Theoretical tools for transport in molecular nanostructures. Physica B: Condensed Matter, 2002, 314, 86-90.	1.3	75
56	Infrared Spectra of Alkylphosphonic Acid Bound to Aluminium Surfaces. Macromolecular Symposia, 2007, 254, 248-253.	0.4	74
57	Graphene-based technologies for energy applications, challenges and perspectives. 2D Materials, 2015, 2, 030204.	2.0	74
58	Controlled Doping of MS₂ (M=W, Mo) Nanotubes and Fullereneâ€like Nanoparticles. Angewandte Chemie - International Edition, 2012, 51, 1148-1151.	7.2	73
59	H₂ Adsorption in Metalâ€Organic Frameworks: Dispersion or Electrostatic Interactions?. Chemistry - A European Journal, 2008, 14, 6597-6600.	1.7	69
60	Planar Tetracoordinate Carbons in Cyclic Hydrocarbons. Organic Letters, 2005, 7, 1509-1512.	2.4	68
61	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	1.1	68
62	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.	8.9	68
63	Atomic-Scale Structure of Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 3928-3931.	4.5	68
64	Hydrogen Adsorption Sites in Zeolite Imidazolate Frameworks ZIF-8 and ZIF-11. Journal of Physical Chemistry C, 2010, 114, 13381-13384.	1.5	66
65	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
66	Concentric-shell fullerenes and diamond particles: A molecular-dynamics study. Physical Review B, 1999, 60, 10711-10714.	1.1	64
67	Nanolubrication: How Do MoS2-Based Nanostructures Lubricate?. Journal of Physical Chemistry C, 2008, 112, 17764-17767.	1.5	64
68	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	0.6	63
69	MoS₂ Hybrid Nanostructures: From Octahedral to Quasiâ€Spherical Shells within Individual Nanoparticles. Angewandte Chemie - International Edition, 2011, 50, 1810-1814.	7.2	62
70	Toward Atomic-Scale Bright-Field Electron Tomography for the Study of Fullerene-Like Nanostructures. Nano Letters, 2008, 8, 891-896.	4.5	61
71	Interfacial Approach toward Benzeneâ€Bridged Polypyrrole Filmâ€“Based Microâ€Supercapacitors with Ultrahigh Volumetric Power Density. Advanced Functional Materials, 2020, 30, 1908243.	7.8	60
72	Hydrogen adsorption by perforated graphene. International Journal of Hydrogen Energy, 2015, 40, 6594-6599.	3.8	59

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73	Adsorption of hydrogen in covalent organic frameworks: Comparison of simulations and experiments. Microporous and Mesoporous Materials, 2010, 133, 59-65.	2.2	58
74	Optical Excitations in Cadmium Sulfide Nanoparticles. Journal of Physical Chemistry C, 2007, 111, 10761-10770.	1.5	57
75	Collision Energy Dependence of Molecular Fusion and Fragmentation inC60++C60Collisions. Physical Review Letters, 1996, 76, 3289-3292.	2.9	55
76	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
77	Synthesis of Coreâ€“Shell Inorganic Nanotubes. Advanced Functional Materials, 2010, 20, 2459-2468.	7.8	54
78	Towards an optimal contact metal for CNTFETs. Nanoscale, 2016, 8, 10240-10251.	2.8	54
79	Optics, Mechanics, and Energetics of Two-Dimensional MoS₂ Nanostructures from a Theoretical Perspective. Accounts of Chemical Research, 2015, 48, 48-55.	7.6	53
80	Luminescent Emission of Excited Rydberg Excitons from Monolayer WSe₂. Nano Letters, 2019, 19, 2464-2471.	4.5	51
81	Porous Graphene Oxide/Diboronic Acid Materials: Structure and Hydrogen Sorption. Journal of Physical Chemistry C, 2015, 119, 27179-27191.	1.5	49
82	Optical Properties of Cadmium Sulfide Clusters. Journal of Physical Chemistry B, 2003, 107, 2897-2902.	1.2	46
83	Electromechanical Switch Based on Mo₆S₆ Nanowires. Nano Letters, 2008, 8, 4093-4097.	4.5	45
84	Hollow V₂O₅ Nanoparticles (Fullerene-Like Analogues) Prepared by Laser Ablation. Journal of the American Chemical Society, 2010, 132, 11214-11222.	6.6	45
85	D5h C50 Fullerene:â€‰ A Building Block for Oligomers and Solids?. Journal of Physical Chemistry A, 2004, 108, 11733-11739.	1.1	42
86	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
87	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
88	Dielectric Properties of Selected Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2014, 118, 11799-11805.	1.5	40
89	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
90	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

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91	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. International Journal of Hydrogen Energy, 2011, 36, 6005-6013.	3.8	38
92	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
93	Vibrational signatures of fullerene oxides. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2287-2294.	1.7	36
94	On the nature of the interaction between H2 and metal-organic frameworks. Theoretical Chemistry Accounts, 2008, 120, 543-550.	0.5	36
95	High resolution TEM study of WS₂ nanotubes. Physica Status Solidi (B): Basic Research, 2011, 248, 2716-2719.	0.7	35
96	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
97	Optical Properties of Triangular Molybdenum Disulfide Nanoflakes. Journal of Physical Chemistry Letters, 2014, 5, 3636-3640.	2.1	35
98	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
99	Curved TiO₂ Nanoparticles in Water: Short (Chemical) and Long (Physical) Range Interfacial Effects. ACS Applied Materials & Interfaces, 2018, 10, 29943-29953.	4.0	35
100	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
101	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
102	Microscopic Investigation of Shear in Multiwalled Nanotube Deformation. Journal of Physical Chemistry C, 2007, 111, 8432-8436.	1.5	33
103	Fullereneâ€like Mo(W)_{1â^'x}Re_xS₂ Nanoparticles. Chemistry - an Asian Journal, 2008, 3, 1568-1574.	1.7	33
104	Curvature effects of nitrogen on graphitic sheets: Structures and energetics. Chemical Physics Letters, 2007, 447, 115-120.	1.2	32
105	Stretching and breaking of monolayer MoS ₂ â€”an atomistic simulation. 2D Materials, 2014, 1, 011007.	2.0	32
106	Hyperdiamond and hyperlonsdaleit: Possible crystalline phases of fullereneC28. Physical Review B, 2005, 72, .	1.1	31
107	C28fulleritesâ€”structure, electronic properties and intercalates. Physical Chemistry Chemical Physics, 2006, 8, 3320-3325.	1.3	31
108	Stability and Electronic Properties of Bismuth Nanotubes. Journal of Physical Chemistry C, 2010, 114, 22092-22097.	1.5	31

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109	Unique Structural and Transport Properties of Molybdenum Chalcohalide Nanowires. Physical Review Letters, 2007, 99, 085503.	2.9	30
110	Localized defect states in MoS₂monolayers: Electronic and optical properties. Physica Status Solidi (B): Basic Research, 2017, 254, 1600645.	0.7	30
111	MonS2n+x clustersâ€"magic numbers and platelets. Computational Materials Science, 2006, 35, 316-320.	1.4	29
112	Nanoseashells and Nanooctahedra of MoS2: Routes to Inorganic Fullerenes. Chemistry of Materials, 2009, 21, 5627-5636.	3.2	29
113	Electronic and magnetic properties of DUT-8(Ni). Physical Chemistry Chemical Physics, 2015, 17, 17122-17129.	1.3	29
114	Nanotube Electromechanics beyond Carbon: The Case of WS₂. ACS Nano, 2015, 9, 12224-12232.	7.3	29
115	Porous graphite oxide pillared with tetrapod-shaped molecules. Carbon, 2017, 120, 145-156.	5.4	29
116	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
117	Hydrogen adsorption sites and energies in 2D and 3D covalent organic frameworks. Chemical Physics Letters, 2010, 489, 86-91.	1.2	27
118	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
119	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
120	Single- to Triple-Wall WS2 Nanotubes Obtained by High-Power Plasma Ablation of WS2 Multiwall Nanotubes. Inorganics, 2014, 2, 177-190.	1.2	27
121	Multilayered intercalation of 1-octanol into Brodie graphite oxide. Nanoscale, 2017, 9, 6929-6936.	2.8	27
122	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
123	Simulation of Inorganic Nanotubes. Springer Series in Materials Science, 2007, , 33-57.	0.4	26
124	Capillary Imbibition of PbI₂ Melt by Inorganic and Carbon Nanotubes. Journal of Physical Chemistry C, 2009, 113, 13664-13669.	1.5	26
125	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
126	An efficient way to model complex magnetite: Assessment of SCC-DFTB against DFT. Journal of Chemical Physics, 2019, 150, 094703.	1.2	24

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127	Tubular structures of germanium. Solid State Communications, 2001, 119, 653-657.	0.9	23
128	Density-functional-based molecular-dynamics simulations of molten salts. Journal of Chemical Physics, 2005, 123, 134510.	1.2	23
129	Catalysts on the edge. Nature Nanotechnology, 2007, 2, 21-22.	15.6	23
130	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
131	Optimizing Electronic Structure and Quantum Transport at the Graphene-Si(111) Interface: AnAbÂInitioDensity-Functional Study. Physical Review Letters, 2013, 110, 176805.	2.9	23
132	Combined SnS@SnS₂double layers: charge transfer and electronic structure. Semiconductor Science and Technology, 2014, 29, 064006.	1.0	23
133	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
134	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
135	Structural and energetic parallels between hydrogenated and fluorinated fullerenes: C36X6. Journal of the Chemical Society Perkin Transactions II, 1999, , 707-712.	0.9	22
136	Physisorption of N2 on graphene platelets: An Ab initio study. International Journal of Quantum Chemistry, 2006, 106, 1375-1382.	1.0	22
137	Adsorption of nucleotides on the rutile (110) surface. International Journal of Materials Research, 2010, 101, 758-764.	0.1	22
138	Polymorphs of lithium-boron imidazolates: energy landscape and hydrogen storage properties. Dalton Transactions, 2011, 40, 3796-3798.	1.6	22
139	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
140	Formation, Structure, and Polymorphism of Novel Lowestâ€Dimensional AgI Nanoaggregates by Encapsulation in Carbon Nanotubes. Small, 2007, 3, 1730-1734.	5.2	21
141	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
142	Car-Parrinello treatment for an approximate density-functional theory method. Journal of Chemical Physics, 2007, 126, 124103.	1.2	19
143	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
144	Prediction of huge magnetic anisotropies of transition-metal dimer-benzene complexes from density functional theory calculations. Physical Review B, 2010, 82, .	1.1	18

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145	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
146	Nanomechanical Energy Storage in Twisted Nanotube Ropes. Physical Review Letters, 2012, 109, 255501.	2.9	18
147	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
148	Molecular Dynamics Study of the Mechanical and Electronic Properties of Carbon Nanotubes. Small, 2005, 1, 399-402.	5.2	16
149	Molecular design of fullerene-based ultralow-kdielectrics. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 3868-3872.	0.8	16
150	Limits of mechanical energy storage and structural changes in twisted carbon nanotube ropes. Physical Review B, 2013, 88, .	1.1	16
151	Toward Activity Origin of Electrocatalytic Hydrogen Evolution Reaction on Carbonâ€Rich Crystalline Coordination Polymers. Small, 2017, 13, 1700783.	5.2	16
152	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
153	Magnetism and the potential energy hypersurfaces of Fe53 to Fe57. Computational Materials Science, 2006, 35, 297-301.	1.4	15
154	Aspects of the Proton Transfer in Liquid Phosphonic Acid. Journal of Physical Chemistry B, 2009, 113, 8475-8480.	1.2	15
155	Graphite oxide swelling in molten sugar alcohols and their aqueous solutions. Carbon, 2018, 140, 157-163.	5.4	15
156	Interlayer Excitons in Transitionâ€Metal Dichalcogenide Heterobilayers. Physica Status Solidi (B): Basic Research, 2019, 256, 1900308.	0.7	15
157	Oneâ€and Twoâ€Dimensional Inorganic Crystals inside Inorganic Nanotubes. European Journal of Inorganic Chemistry, 2010, 2010, 4233-4243.	1.0	14
158	Experimental, finite element, and density-functional theory study of inorganic nanotube compression. Applied Physics Letters, 2011, 98, 081908.	1.5	14
159	Two-dimensional and tubular structures of misfit compounds: Structural and electronic properties. Beilstein Journal of Nanotechnology, 2014, 5, 2171-2178.	1.5	14
160	Is MoS2a robust material for 2D electronics?. Nanotechnology, 2014, 25, 445201.	1.3	14
161	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
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