Thomas Heine

List of Publications by Year
in descending order

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394	32,673	2963	4978
papers	citations	93 h-index	167 g-index

438	438	438	28586
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Influence of quantum confinement on the electronic structure of the transition metal sulfide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>T</mml:mi></mml:mrow></mml:math>S<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical	1.1	1,474
2	Construction of Crystalline 2D Covalent Organic Frameworks with Remarkable Chemical (Acid/Base) Stability via a Combined Reversible and Irreversible Route. Journal of the American Chemical Society, 2012, 134, 19524-19527.	6.6	1,442
3	An atlas of two-dimensional materials. Chemical Society Reviews, 2014, 43, 6537-6554.	18.7	1,159
4	Two-dimensional sp ² carbonâ€“conjugated covalent organic frameworks. Science, 2017, 357, 673-676.	6.0	866
5	Mechanochemical Synthesis of Chemically Stable Isoreticular Covalent Organic Frameworks. Journal of the American Chemical Society, 2013, 135, 5328-5331.	6.6	821
6	Chemically Stable Multilayered Covalent Organic Nanosheets from Covalent Organic Frameworks via Mechanical Delamination. Journal of the American Chemical Society, 2013, 135, 17853-17861.	6.6	717
7	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
8	Mixed Matrix Membranes (MMMs) Comprising Exfoliated 2D Covalent Organic Frameworks (COFs) for Efficient CO₂ Separation. Chemistry of Materials, 2016, 28, 1277-1285.	3.2	541
9	Chemical sensing in two dimensional porous covalent organic nanosheets. Chemical Science, 2015, 6, 3931-3939.	3.7	504
10	Highly Emissive Covalent Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 5797-5800.	6.6	501
11	Induced magnetic fields in aromatic [n]-annulenesâ€”interpretation of NICS tensor components. Physical Chemistry Chemical Physics, 2004, 6, 273-276.	1.3	425
12	Enhancement of Chemical Stability and Crystallinity in Porphyrinâ€Containing Covalent Organic Frameworks by Intramolecular Hydrogen Bonds. Angewandte Chemie - International Edition, 2013, 52, 13052-13056.	7.2	411
13	A stable non-classical metallofullerene family. Nature, 2000, 408, 427-428.	13.7	379
14	High-mobility band-like charge transport in a semiconducting two-dimensional metalâ€“organic framework. Nature Materials, 2018, 17, 1027-1032.	13.3	341
15	GeP₃: A Small Indirect Band Gap 2D Crystal with High Carrier Mobility and Strong Interlayer Quantum Confinement. Nano Letters, 2017, 17, 1833-1838.	4.5	338
16	Two-Dimensional Cu₂Si Monolayer with Planar Hexacoordinate Copper and Silicon Bonding. Journal of the American Chemical Society, 2015, 137, 2757-2762.	6.6	335
17	Solid state organic amine detection in a photochromic porous metal organic framework. Chemical Science, 2015, 6, 1420-1425.	3.7	316
18	Interplaying Intrinsic and Extrinsic Proton Conductivities in Covalent Organic Frameworks. Chemistry of Materials, 2016, 28, 1489-1494.	3.2	310

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19	Molecular Level Control of the Capacitance of Two-Dimensional Covalent Organic Frameworks: Role of Hydrogen Bonding in Energy Storage Materials. Chemistry of Materials, 2017, 29, 2074-2080.	3.2	277
20	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
21	A Nitrogenâ€Rich 2D sp²â€Carbonâ€Linked Conjugated Polymer Framework as a Highâ€Performance Cathode for Lithiumâ€Ion Batteries. Angewandte Chemie - International Edition, 2019, 58, 849-853.	7.2	275
22	The Induced Magnetic Field in Cyclic Molecules. Chemistry - A European Journal, 2004, 10, 4367-4371.	1.7	266
23	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
24	Transition Metal Chalcogenides: Ultrathin Inorganic Materials with Tunable Electronic Properties. Accounts of Chemical Research, 2015, 48, 65-72.	7.6	262
25	On-water surface synthesis of crystalline, few-layer two-dimensional polymers assisted by surfactant monolayers. Nature Chemistry, 2019, 11, 994-1000.	6.6	262
26	Strain-dependent modulation of conductivity in single-layer transition-metal dichalcogenides. Physical Review B, 2013, 87, .	1.1	255
27	Stacking in Bulk and Bilayer Hexagonal Boron Nitride. Physical Review Letters, 2013, 111, 036104.	2.9	252
28	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS₂ Nanoribbons. Journal of Physical Chemistry Letters, 2012, 3, 2934-2941.	2.1	229
29	Multiple-component covalent organic frameworks. Nature Communications, 2016, 7, 12325.	5.8	227
30	Unveiling Electronic Properties in Metalâ€“Phthalocyanine-Based Pyrazine-Linked Conjugated Two-Dimensional Covalent Organic Frameworks. Journal of the American Chemical Society, 2019, 141, 16810-16816.	6.6	227
31	Ionic Covalent Organic Frameworks: Design of a Charged Interface Aligned on 1D Channel Walls and Its Unusual Electrostatic Functions. Angewandte Chemie - International Edition, 2017, 56, 4982-4986.	7.2	217
32	Two Dimensional Materials Beyond MoS₂: Nobleâ€Transitionâ€Metal Dichalcogenides. Angewandte Chemie - International Edition, 2014, 53, 3015-3018.	7.2	215
33	Recent advances in planar tetracoordinate carbon chemistry. Journal of Computational Chemistry, 2007, 28, 362-372.	1.5	211
34	Photoinduced Chargeâ€Carrier Generation in Epitaxial MOF Thin Films: High Efficiency as a Result of an Indirect Electronic Band Gap?. Angewandte Chemie - International Edition, 2015, 54, 7441-7445.	7.2	206
35	The Induced Magnetic Field. Accounts of Chemical Research, 2012, 45, 215-228.	7.6	204
36	The electronic structure calculations of two-dimensional transition-metal dichalcogenides in the presence of external electric and magnetic fields. Chemical Society Reviews, 2015, 44, 2603-2614.	18.7	204

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37	The Structure of Layered Covalentâ€Organic Frameworks. Chemistry - A European Journal, 2011, 17, 2388-2392.	1.7	203
38	Extension of the Universal Force Field to Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 880-891.	2.3	200
39	Ultrastable Imineâ€Based Covalent Organic Frameworks for Sulfuric Acid Recovery: An Effect of Interlayer Hydrogen Bonding. Angewandte Chemie - International Edition, 2018, 57, 5797-5802.	7.2	192
40	A novel series of isoreticular metal organic frameworks: realizing metastable structures by liquid phase epitaxy. Scientific Reports, 2012, 2, 921.	1.6	183
41	The Magnetic Shielding Function of Molecules and Pi-Electron Delocalization. Chemical Reviews, 2005, 105, 3889-3910.	23.0	182
42	Pentagon adjacency as a determinant of fullerene stability. Physical Chemistry Chemical Physics, 1999, 1, 2913-2918.	1.3	178
43	Density-functional based tight-binding: an approximate DFT method. Journal of the Brazilian Chemical Society, 2009, 20, 1193-1205.	0.6	177
44	Imogolite Nanotubes: Stability, Electronic, and Mechanical Properties. ACS Nano, 2007, 1, 362-368.	7.3	172
45	Two-Dimensional Topological Insulators: Progress and Prospects. Journal of Physical Chemistry Letters, 2017, 8, 1905-1919.	2.1	170
46	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
47	Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation. Angewandte Chemie - International Edition, 2016, 55, 7806-7810.	7.2	168
48	Borazine: to be or not to be aromatic. Structural Chemistry, 2007, 18, 833-839.	1.0	167
49	Robust Two-Dimensional Topological Insulators in Methyl-Functionalized Bismuth, Antimony, and Lead Bilayer Films. Nano Letters, 2015, 15, 1083-1089.	4.5	166
50	Highly oriented MOF thin film-based electrocatalytic device for the reduction of CO₂ to CO exhibiting high faradaic efficiency. Journal of Materials Chemistry A, 2016, 4, 15320-15326.	5.2	166
51	B₁₉^{â^'}: An Aromatic Wankel Motor. Angewandte Chemie - International Edition, 2010, 49, 5668-5671.	7.2	162
52	Description of Electron Delocalization via the Analysis of Molecular Fields. Chemical Reviews, 2005, 105, 3812-3841.	23.0	160
53	Photocarrier generation from interlayer charge-transfer transitions in WS ₂ -graphene heterostructures. Science Advances, 2018, 4, e1700324.	4.7	160
54	Precise and reversible band gap tuning in single-layer MoSe₂ by uniaxial strain. Nanoscale, 2016, 8, 2589-2593.	2.8	159

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55	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
56	MFUâ€4 â€“ A Metalâ€Organic Framework for Highly Effective H₂/D₂ Separation. Advanced Materials, 2013, 25, 635-639.	11.1	150
57	Control of biaxial strain in single-layer molybdenite using local thermal expansion of the substrate. 2D Materials, 2015, 2, 015006.	2.0	149
58	Colloidal Synthesis of Single-Layer MSe₂ (M = Mo, W) Nanosheets via Anisotropic Solution-Phase Growth Approach. Journal of the American Chemical Society, 2015, 137, 7266-7269.	6.6	147
59	Interaction of Small Gases with the Unsaturated Metal Centers of the HKUST-1 Metal Organic Framework. Journal of Physical Chemistry C, 2013, 117, 14570-14578.	1.5	145
60	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
61	Electromechanics in MoS2 and WS2: nanotubes vs. monolayers. Scientific Reports, 2013, 3, 2961.	1.6	142
62	Transitionâ€metal dichalcogenides for spintronic applications. Annalen Der Physik, 2014, 526, 395-401.	0.9	140
63	On the reticular construction concept of covalent organic frameworks. Beilstein Journal of Nanotechnology, 2010, 1, 60-70.	1.5	139
64	Tandem intercalation strategy for single-layer nanosheets as an effective alternative to conventional exfoliation processes. Nature Communications, 2015, 6, 5763.	5.8	137
65	Highly Effective Hydrogen Isotope Separation in Nanoporous Metalâ€“Organic Frameworks with Open Metal Sites: Direct Measurement and Theoretical Analysis. ACS Nano, 2014, 8, 761-770.	7.3	135
66	Engineering crystalline quasi-two-dimensional polyaniline thin film with enhanced electrical and chemiresistive sensing performances. Nature Communications, 2019, 10, 4225.	5.8	132
67	Do All-Metal Antiaromatic Clusters Exist?. Journal of the American Chemical Society, 2003, 125, 13930-13931.	6.6	131
68	Nanoporous Designer Solids with Huge Lattice Constant Gradients: Multiheteroepitaxy of Metalâ€“Organic Frameworks. Nano Letters, 2014, 14, 1526-1529.	4.5	130
69	Boron Rings Enclosing Planar Hypercoordinate Group 14 Elements. Journal of the American Chemical Society, 2007, 129, 14767-14774.	6.6	129
70	Theoretical Analysis of the Smallest Carbon Cluster Containing a Planar Tetracoordinate Carbon. Journal of the American Chemical Society, 2004, 126, 16160-16169.	6.6	126
71	Extension of the Universal Force Field for Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2016, 12, 5215-5225.	2.3	126
72	Highly Sensitive Electromechanical Piezoresistive Pressure Sensors Based on Large-Area Layered PtSe₂ Films. Nano Letters, 2018, 18, 3738-3745.	4.5	125

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73	Defects in MOFs: A Thorough Characterization. ChemPhysChem, 2012, 13, 2025-2029.	1.0	121
74	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. Chemical Communications, 2011, 47, 6242.	2.2	120
75	3D Synergistically Active Carbon Nanofibers for Improved Oxygen Evolution. Advanced Energy Materials, 2017, 7, 1602928.	10.2	120
76	Ïƒ and Ï€ contributions to the induced magnetic field: Indicators for the mobility of electrons in molecules. Journal of Computational Chemistry, 2007, 28, 302-309.	1.5	119
77	A semiconducting layered metal-organic framework magnet. Nature Communications, 2019, 10, 3260.	5.8	119
78	DFTB Parameters for the Periodic Table: Part 1, Electronic Structure. Journal of Chemical Theory and Computation, 2013, 9, 4006-4017.	2.3	117
79	Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides. Physical Review B, 2015, 92, .	1.1	117
80	Fabrication of Highly Uniform Gel Coatings by the Conversion of Surface-Anchored Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 8-11.	6.6	116
81	Twoâ€Ðimensional Boronate Ester Covalent Organic Framework Thin Films with Large Single Crystalline Domains for a Neuromorphic Memory Device. Angewandte Chemie - International Edition, 2020, 59, 8218-8224.	7.2	116
82	High-Mobility Semiconducting Two-Dimensional Conjugated Covalent Organic Frameworks with p-Type Doping. Journal of the American Chemical Society, 2020, 142, 21622-21627.	6.6	113
83	The Rise of Two-Dimensional Materials. Accounts of Chemical Research, 2015, 48, 1-2.	7.6	111
84	Ïƒ-Antiaromaticity in Cyclobutane, Cubane, and Other Molecules with Saturated Four-Membered Rings. Organic Letters, 2003, 5, 23-26.	2.4	108
85	B₁₈^{2â^'}: a quasi-planar bowl member of the Wankel motor family. Chemical Communications, 2014, 50, 8140-8143.	2.2	107
86	Transition-metal dichalcogenide bilayers: Switching materials for spintronic and valleytronic applications. Physical Review B, 2014, 90, .	1.1	105
87	Study of angiotensin-(1â€“7) vasoactive peptide and its Î²-cyclodextrin inclusion complexes: Complete sequence-specific NMR assignments and structural studies. Peptides, 2007, 28, 2199-2210.	1.2	104
88	CAl4Be and CAl3Be2â^': global minima with a planar pentacoordinate carbon atom. Chemical Communications, 2010, 46, 8776.	2.2	104
89	Evaluation of aromaticity: A new dissected NICS model based on canonical orbitals. Physical Chemistry Chemical Physics, 2003, 5, 246-251.	1.3	100
90	Density Functional Theory and Beyond for Band-Gap Screening: Performance for Transition-Metal Oxides and Dichalcogenides. Journal of Chemical Theory and Computation, 2013, 9, 2950-2958.	2.3	99

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91	Capture of heavy hydrogen isotopes in a metal-organic framework with active Cu(I) sites. Nature Communications, 2017, 8, 14496.	5.8	98
92	Highly Crystalline and Semiconducting Imineâ€Based Twoâ€Dimensional Polymers Enabled by Interfacial Synthesis. Angewandte Chemie - International Edition, 2020, 59, 6028-6036.	7.2	98
93	Spontaneous Ripple Formation in MoS₂ Monolayers: Electronic Structure and Transport Effects. Advanced Materials, 2013, 25, 5473-5475.	11.1	97
94	Revealing unusual chemical bonding in planar hyper-coordinate Ni₂Ge and quasi-planar Ni₂Si two-dimensional crystals. Physical Chemistry Chemical Physics, 2015, 17, 26043-26048.	1.3	95
95	PtTe Monolayer: Two-Dimensional Electrocatalyst with High Basal Plane Activity toward Oxygen Reduction Reaction. Journal of the American Chemical Society, 2018, 140, 12732-12735.	6.6	95
96	Identification of Prime Factors to Maximize the Photocatalytic Hydrogen Evolution of Covalent Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 9752-9762.	6.6	94
97	C36, a hexavalent building block for fullerene compounds and solids. Chemical Physics Letters, 1999, 300, 369-378.	1.2	93
98	Hydrogen Sieving and Storage in Fullerene Intercalated Graphite. Nano Letters, 2007, 7, 1-5.	4.5	92
99	Theoretical Studies on the Smallest Fullerene: from Monomer to Oligomers and Solid States. Chemistry - A European Journal, 2004, 10, 963-970.	1.7	90
100	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
101	Structure and Fluxionality of B₁₃⁺ Probed by Infrared Photodissociation Spectroscopy. Angewandte Chemie - International Edition, 2017, 56, 501-504.	7.2	88
102	Two-Dimensional Kagome Lattices Made of Hetero Triangulenes Are Dirac Semimetals or Single-Band Semiconductors. Journal of the American Chemical Society, 2019, 141, 743-747.	6.6	88
103	Polyoxometalates Made of Gold: The Polyoxoaurate [Au^{III}₄As^V₄O₂₀]^{8â^'}. Angewandte Chemie - International Edition, 2010, 49, 1886-1889.	7.2	87
104	Aromaticity of Four-Membered-Ring 6Ï€-Electron Systems:â€‰ N2S2 and Li2C4H4. Journal of the American Chemical Society, 2004, 126, 3132-3138.	6.6	86
105	Noncovalent Bifunctional Organocatalysts: Powerful Tools for Contiguous Quaternaryâ€Tertiary Stereogenic Carbon Formation, Scope, and Origin of Enantioselectivity. Chemistry - A European Journal, 2012, 18, 4088-4098.	1.7	86
106	A Singleâ€Material Logical Junction Based on 2D Crystal PdS₂. Advanced Materials, 2016, 28, 853-856.	11.1	85
107	Energetics of Fullerenes with Four-Membered Rings. The Journal of Physical Chemistry, 1996, 100, 6984-6991.	2.9	84
108	Boronâ€“nitrogen analogues of the fullerenes: the isolated-square rule. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2197-2201.	1.7	84

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109	Antiaromaticity in Bare Deltahedral Silicon Clusters Satisfying Wade's and Hirsch's Rules:Â An Apparent Correlation of Antiaromaticity with High Symmetry. Journal of the American Chemical Society, 2004, 126, 430-431.	6.6	82
110	Highly accessible and dense surface single metal FeN₄ active sites for promoting the oxygen reduction reaction. Energy and Environmental Science, 2022, 15, 2619-2628.	15.6	82
111	Dynamical behavior of Borospherene: A Nanobubble. Scientific Reports, 2015, 5, 11287.	1.6	81
112	Post-anti-van't Hoff-Le Bel motif in atomically thin germaniumâ€“copper alloy film. Physical Chemistry Chemical Physics, 2015, 17, 17545-17551.	1.3	81
113	Fluxional Boron Clusters: From Theory to Reality. Accounts of Chemical Research, 2019, 52, 2732-2744.	7.6	79
114	Twoâ€Dimensional Nobleâ€Metal Chalcogenides and Phosphochalcogenides. Angewandte Chemie - International Edition, 2020, 59, 9242-9254.	7.2	78
115	Structural and electronic properties of graphene nanoflakes. Physical Review B, 2010, 81, .	1.1	77
116	Electronic properties of transition-metal dichalcogenides. MRS Bulletin, 2015, 40, 577-584.	1.7	77
117	Topological two-dimensional polymers. Chemical Society Reviews, 2020, 49, 2007-2019.	18.7	76
118	Poly(perfluoroalkylation) of Metallic Nitride Fullerenes Reveals Addition-Pattern Guidelines: Synthesis and Characterization of a Family of Sc₃N@C₈₀(CF₃)_n(n= 2â^’16) and Their Radical Anions. Journal of the American Chemical Society, 2011, 133, 2672-2690.	6.6	73
119	Single-Layer Tl₂O: A Metal-Shrouded 2D Semiconductor with High Electronic Mobility. Journal of the American Chemical Society, 2017, 139, 11694-11697.	6.6	72
120	A Nitrogenâ€Rich 2D sp²â€Carbonâ€Linked Conjugated Polymer Framework as a Highâ€Performance Cathode for Lithiumâ€Ion Batteries. Angewandte Chemie, 2019, 131, 859-863.	1.6	71
121	Porous Dithiine-Linked Covalent Organic Framework as a Dynamic Platform for Covalent Polysulfide Anchoring in Lithiumâ€“Sulfur Battery Cathodes. Journal of the American Chemical Society, 2022, 144, 9101-9112.	6.6	71
122	What Is the Maximum Coordination Number in a Planar Structure?. Angewandte Chemie - International Edition, 2012, 51, 4275-4276.	7.2	70
123	H₂ Adsorption in Metalâ€Organic Frameworks: Dispersion or Electrostatic Interactions?. Chemistry - A European Journal, 2008, 14, 6597-6600.	1.7	69
124	Planar Tetracoordinate Carbons in Cyclic Hydrocarbons. Organic Letters, 2005, 7, 1509-1512.	2.4	68
125	Visualizing electronic interactions between iron and carbon by X-ray chemical imaging and spectroscopy. Chemical Science, 2015, 6, 3262-3267.	3.7	68
126	Two-dimensional ferroelastic topological insulators in single-layer Janus transition metal dichalcogenides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>M</mml:mi><mml:mi>SSe</mml:mi></mml:mrow></mml:m	1.1	68

Physical Review B, 2018, 98, .

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127	From layers to nanotubes: Transition metal disulfides TMS2. European Physical Journal B, 2012, 85, 1.	0.6	67
128	AuToGraFS: Automatic Topological Generator for Framework Structures. Journal of Physical Chemistry A, 2014, 118, 9607-9614.	1.1	67
129	Dynamical behavior of boron clusters. Nanoscale, 2016, 8, 17639-17644.	2.8	67
130	Structure and bonding of IrB₁₂^{â^'}: converting a rigid boron B₁₂ platelet to a Wankel motor. RSC Advances, 2016, 6, 27177-27182.	1.7	67
131	Ultrathin Layers of PdPX (X=S, Se): Two Dimensional Semiconductors for Photocatalytic Water Splitting. Chemistry - A European Journal, 2017, 23, 13612-13616.	1.7	66
132	Energetics of fullerenes with heptagonal rings. Journal of the Chemical Society, Faraday Transactions, 1996, 92, 2203.	1.7	65
133	A Nobleâ€Metalate Bowl: The Polyoxoâ€6â€vanado(V)â€7â€palladate(II) [Pd₇V₆O₂₄(OH)₂]^{6â^'}. Angewandte Chemie - International Edition, 2010, 49, 7807-7811.	7.2	65
134	Room temperature quantum spin Hall states in two-dimensional crystals composed of pentagonal rings and their quantum wells. NPG Asia Materials, 2016, 8, e264-e264.	3.8	65
135	Nanolubrication: How Do MoS2-Based Nanostructures Lubricate?. Journal of Physical Chemistry C, 2008, 112, 17764-17767.	1.5	64
136	Proximity Effect in Crystalline Framework Materials: Stackingâ€Induced Functionality in MOFs and COFs. Advanced Functional Materials, 2020, 30, 1908004.	7.8	64
137	Structural and Electronic Properties of Bulk Gibbsite and Gibbsite Surfaces. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2005, 631, 1267-1271.	0.6	63
138	On the Mechanism of Hydrogen Activation by Frustrated Lewis Pairs. Chemistry - A European Journal, 2013, 19, 17413-17424.	1.7	62
139	Two-dimensional inversion-asymmetric topological insulators in functionalized III-Bi bilayers. Physical Review B, 2015, 91, .	1.1	60
140	Cavitation energies can outperform dispersion interactions. Nature Chemistry, 2018, 10, 1252-1257.	6.6	60
141	(NHC^{Me})SiCl₄: a versatile carbene transfer reagent â€“ synthesis from silicochloroform. Chemical Science, 2013, 4, 77-83.	3.7	59
142	2D Honeycombâ€Kagome Polymer Tandem as Effective Metalâ€Free Photocatalysts for Water Splitting. Advanced Materials, 2021, 33, e2008645.	11.1	57
143	Two-dimensional transition metal dichalcogenides with a hexagonal lattice: Room-temperature quantum spin Hall insulators. Physical Review B, 2016, 93, .	1.1	56
144	Defect Healing and Charge Transfer-Mediated Valley Polarization in MoS₂/MoSe₂/MoS₂ Trilayer van der Waals Heterostructures. Nano Letters, 2017, 17, 4130-4136.	4.5	56

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145	A Tight-Binding Treatment for13C NMR Spectra of Fullerenes. Journal of Physical Chemistry A, 1999, 103, 8738-8746.	1.1	55
146	CBe5Eâ‾ (E = Al, Ga, In, Tl): planar pentacoordinate carbon in heptaatomic clusters. Physical Chemistry Chemical Physics, 2012, 14, 14764.	1.3	55
147	DFTB Parameters for the Periodic Table, Part 2: Energies and Energy Gradients from Hydrogen to Calcium. Journal of Chemical Theory and Computation, 2015, 11, 5209-5218.	2.3	55
148	Dissolving uptake-hindering surface defects in metalâ€“organic frameworks. Chemical Science, 2019, 10, 153-160.	3.7	55
149	Crystal size versus paddle wheel deformability: selective gated adsorption transitions of the switchable metalâ€“organic frameworks DUT-8(Co) and DUT-8(Ni). Journal of Materials Chemistry A, 2019, 7, 21459-21475.	5.2	54
150	13C NMR fingerprint characterizes long time-scale structure of Sc3N@C80 endohedral fullerene. Magnetic Resonance in Chemistry, 2004, 42, S199-S201.	1.1	53
151	Structure and Electron Delocalization in Al42- and Al44-. Journal of Chemical Theory and Computation, 2007, 3, 775-781.	2.3	53
152	Palladastannatrane - a PdIIâ†'SnIVDative Bond. European Journal of Inorganic Chemistry, 2008, 2008, 4225-4229.	1.0	52
153	And Yet It Rotates: The Starter for a Molecular Wankel Motor. Angewandte Chemie - International Edition, 2012, 51, 10226-10227.	7.2	51
154	Large-grain MBE-grown GaSe on GaAs with a Mexican hat-like valence band dispersion. Npj 2D Materials and Applications, 2018, 2, .	3.9	51
155	Two-dimensional Pd₃P₂S₈ semiconductors as photocatalysts for the solar-driven oxygen evolution reaction: a theoretical investigation. Journal of Materials Chemistry A, 2018, 6, 23495-23501.	5.2	51
156	Highâ€Precision Size Recognition and Separation in Synthetic 1D Nanochannels. Angewandte Chemie - International Edition, 2019, 58, 15922-15927.	7.2	50
157	Raman spectroscopy studies of the terahertz vibrational modes of a DUT-8 (Ni) metalâ€“organic framework. Physical Chemistry Chemical Physics, 2017, 19, 32099-32104.	1.3	49
158	Cation-selective two-dimensional polyimine membranes for high-performance osmotic energy conversion. Nature Communications, 2022, 13, .	5.8	49
159	Ab Initio Study of the Adsorption of Small Molecules on Metalâ€“Organic Frameworks with Oxo-centered Trimetallic Building Units: The Role of the Undercoordinated Metal Ion. Inorganic Chemistry, 2015, 54, 8251-8263.	1.9	48
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