

# Thomas Heine

## List of Publications by Citations

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382  
papers

24,876  
citations

85  
h-index

146  
g-index

438  
ext. papers

28,668  
ext. citations

8.4  
avg, IF

7.42  
L-index

#	Paper	IF	Citations
382	Influence of quantum confinement on the electronic structure of the transition metal sulfide TS2. <i>Physical Review B</i> , <b>2011</b> , 83,	3.3	1247
381	Construction of crystalline 2D covalent organic frameworks with remarkable chemical (acid/base) stability via a combined reversible and irreversible route. <i>Journal of the American Chemical Society</i> , <b>2012</b> , 134, 19524-7	16.4	939
380	An atlas of two-dimensional materials. <i>Chemical Society Reviews</i> , <b>2014</b> , 43, 6537-54	58.5	905
379	Mechanochemical synthesis of chemically stable isorecticular covalent organic frameworks. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 5328-31	16.4	555
378	Two-dimensional sp carbon-conjugated covalent organic frameworks. <i>Science</i> , <b>2017</b> , 357, 673-676	33.3	543
377	Chemically stable multilayered covalent organic nanosheets from covalent organic frameworks via mechanical delamination. <i>Journal of the American Chemical Society</i> , <b>2013</b> , 135, 17853-61	16.4	496
376	Graphene nanostructures as tunable storage media for molecular hydrogen. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2005</b> , 102, 10439-44	11.5	487
375	Mixed Matrix Membranes (MMMs) Comprising Exfoliated 2D Covalent Organic Frameworks (COFs) for Efficient CO <sub>2</sub> Separation. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 1277-1285	9.6	404
374	Induced magnetic fields in aromatic [n]-annulenes Interpretation of NICS tensor components. <i>Physical Chemistry Chemical Physics</i> , <b>2004</b> , 6, 273-276	3.6	397
373	Chemical sensing in two dimensional porous covalent organic nanosheets. <i>Chemical Science</i> , <b>2015</b> , 6, 3931-3939	9.4	385
372	Highly Emissive Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 5797-800	16.4	373
371	A stable non-classical metallofullerene family. <i>Nature</i> , <b>2000</b> , 408, 427-8	50.4	354
370	Enhancement of chemical stability and crystallinity in porphyrin-containing covalent organic frameworks by intramolecular hydrogen bonds. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 13052-6	16.4	308
369	Solid state organic amine detection in a photochromic porous metal organic framework. <i>Chemical Science</i> , <b>2015</b> , 6, 1420-1425	9.4	261
368	An Efficient a Posteriori Treatment for Dispersion Interaction in Density-Functional-Based Tight Binding. <i>Journal of Chemical Theory and Computation</i> , <b>2005</b> , 1, 841-7	6.4	251
367	Two-dimensional Cu <sub>2</sub> Si monolayer with planar hexacoordinate copper and silicon bonding. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 2757-62	16.4	237
366	The induced magnetic field in cyclic molecules. <i>Chemistry - A European Journal</i> , <b>2004</b> , 10, 4367-71	4.8	236

365	On the mechanical behavior of WS <sub>2</sub> nanotubes under axial tension and compression. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2006</b> , 103, 523-8	11.5	233
364	GeP: A Small Indirect Band Gap 2D Crystal with High Carrier Mobility and Strong Interlayer Quantum Confinement. <i>Nano Letters</i> , <b>2017</b> , 17, 1833-1838	11.5	228
363	High-mobility band-like charge transport in a semiconducting two-dimensional metal-organic framework. <i>Nature Materials</i> , <b>2018</b> , 17, 1027-1032	27	216
362	Interplaying Intrinsic and Extrinsic Proton Conductivities in Covalent Organic Frameworks. <i>Chemistry of Materials</i> , <b>2016</b> , 28, 1489-1494	9.6	211
361	Strain-dependent modulation of conductivity in single-layer transition-metal dichalcogenides. <i>Physical Review B</i> , <b>2013</b> , 87,	3.3	208
360	Transition metal chalcogenides: ultrathin inorganic materials with tunable electronic properties. <i>Accounts of Chemical Research</i> , <b>2015</b> , 48, 65-72	24.3	203
359	Tuning Magnetism and Electronic Phase Transitions by Strain and Electric Field in Zigzag MoS <sub>2</sub> Nanoribbons. <i>Journal of Physical Chemistry Letters</i> , <b>2012</b> , 3, 2934-41	6.4	203
358	Stacking in bulk and bilayer hexagonal boron nitride. <i>Physical Review Letters</i> , <b>2013</b> , 111, 036104	7.4	202
357	Molecular Level Control of the Capacitance of Two-Dimensional Covalent Organic Frameworks: Role of Hydrogen Bonding in Energy Storage Materials. <i>Chemistry of Materials</i> , <b>2017</b> , 29, 2074-2080	9.6	188
356	Two dimensional materials beyond MoS <sub>2</sub> : noble-transition-metal dichalcogenides. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 3015-8	16.4	183
355	Photoinduced Charge-Carrier Generation in Epitaxial MOF Thin Films: High Efficiency as a Result of an Indirect Electronic Band Gap?. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 7441-5	16.4	182
354	Recent advances in planar tetracoordinate carbon chemistry. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 362-72	3.5	172
353	The induced magnetic field. <i>Accounts of Chemical Research</i> , <b>2012</b> , 45, 215-28	24.3	170
352	The structure of layered covalent-organic frameworks. <i>Chemistry - A European Journal</i> , <b>2011</b> , 17, 2388-924.8	16.4	167
351	Pentagon adjacency as a determinant of fullerene stability. <i>Physical Chemistry Chemical Physics</i> , <b>1999</b> , 1, 2913-2918	3.6	167
350	Ionic Covalent Organic Frameworks: Design of a Charged Interface Aligned on 1D Channel Walls and Its Unusual Electrostatic Functions. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 4982-4986	16.4	166
349	A Nitrogen-Rich 2D sp <sup>2</sup> -Carbon-Linked Conjugated Polymer Framework as a High-Performance Cathode for Lithium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 849-853	16.4	164
348	The magnetic shielding function of molecules and pi-electron delocalization. <i>Chemical Reviews</i> , <b>2005</b> , 105, 3889-910	68.1	163

347	Hydrogen storage by physisorption on nanostructured graphite platelets. <i>Physical Chemistry Chemical Physics</i> , <b>2004</b> , 6, 980	3.6	154
346	A novel series of isorecticular metal organic frameworks: realizing metastable structures by liquid phase epitaxy. <i>Scientific Reports</i> , <b>2012</b> , 2, 921	4.9	153
345	The electronic structure calculations of two-dimensional transition-metal dichalcogenides in the presence of external electric and magnetic fields. <i>Chemical Society Reviews</i> , <b>2015</b> , 44, 2603-14	58.5	149
344	On-water surface synthesis of crystalline, few-layer two-dimensional polymers assisted by surfactant monolayers. <i>Nature Chemistry</i> , <b>2019</b> , 11, 994-1000	17.6	149
343	Imogolite nanotubes: stability, electronic, and mechanical properties. <i>ACS Nano</i> , <b>2007</b> , 1, 362-8	16.7	148
342	Multiple-component covalent organic frameworks. <i>Nature Communications</i> , <b>2016</b> , 7, 12325	17.4	147
341	Borazine: to be or not to be aromatic. <i>Structural Chemistry</i> , <b>2007</b> , 18, 833-839	1.8	147
340	Density-functional based tight-binding: an approximate DFT method. <i>Journal of the Brazilian Chemical Society</i> , <b>2009</b> , 20, 1193-1205	1.5	146
339	Robust two-dimensional topological insulators in methyl-functionalized bismuth, antimony, and lead bilayer films. <i>Nano Letters</i> , <b>2015</b> , 15, 1083-9	11.5	145
338	B19-: an aromatic Wankel motor. <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 5668-71	16.4	145
337	Description of electron delocalization via the analysis of molecular fields. <i>Chemical Reviews</i> , <b>2005</b> , 105, 3812-41	68.1	144
336	Analysis of Aromatic Delocalization: Individual Molecular Orbital Contributions to Nucleus-Independent Chemical Shifts. <i>Journal of Physical Chemistry A</i> , <b>2003</b> , 107, 6470-6475	2.8	141
335	Extension of the Universal Force Field to Metal-Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 880-91	6.4	130
334	Colloidal synthesis of single-layer MSe <sub>2</sub> (M = Mo, W) nanosheets via anisotropic solution-phase growth approach. <i>Journal of the American Chemical Society</i> , <b>2015</b> , 137, 7266-9	16.4	127
333	Defect-induced conductivity anisotropy in MoS <sub>2</sub> monolayers. <i>Physical Review B</i> , <b>2013</b> , 88,	3.3	126
332	Do all-metal antiaromatic clusters exist?. <i>Journal of the American Chemical Society</i> , <b>2003</b> , 125, 13930-1	16.4	124
331	Electromechanics in MoS <sub>2</sub> and WS <sub>2</sub> nanotubes vs. monolayers. <i>Scientific Reports</i> , <b>2013</b> , 3, 2961	4.9	122
330	Highly oriented MOF thin film-based electrocatalytic device for the reduction of CO <sub>2</sub> to CO exhibiting high faradaic efficiency. <i>Journal of Materials Chemistry A</i> , <b>2016</b> , 4, 15320-15326	13	121

329	Boron rings enclosing planar hypercoordinate group 14 elements. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 14767-74	16.4	121
328	Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation. <i>Angewandte Chemie - International Edition</i> , <b>2016</b> , 55, 7806-10	16.4	121
327	Interaction of Small Gases with the Unsaturated Metal Centers of the HKUST-1 Metal Organic Framework. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 14570-14578	3.8	119
326	Ultrastable Imine-Based Covalent Organic Frameworks for Sulfuric Acid Recovery: An Effect of Interlayer Hydrogen Bonding. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 5797-5802	16.4	118
325	Transition-metal dichalcogenides for spintronic applications. <i>Annalen Der Physik</i> , <b>2014</b> , 526, 395-401	2.6	116
324	Photocarrier generation from interlayer charge-transfer transitions in WS-graphene heterostructures. <i>Science Advances</i> , <b>2018</b> , 4, e1700324	14.3	115
323	MFU-4 -- a metal-organic framework for highly effective H(2)/D(2) separation. <i>Advanced Materials</i> , <b>2013</b> , 25, 635-9	24	114
322	Theoretical analysis of the smallest carbon cluster containing a planar tetracoordinate carbon. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 16160-9	16.4	114
321	3D Synergistically Active Carbon Nanofibers for Improved Oxygen Evolution. <i>Advanced Energy Materials</i> , <b>2017</b> , 7, 1602928	21.8	111
320	Two-Dimensional Topological Insulators: Progress and Prospects. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 1905-1919	6.4	110
319	Nanoporous designer solids with huge lattice constant gradients: multiheteroepitaxy of metal-organic frameworks. <i>Nano Letters</i> , <b>2014</b> , 14, 1526-9	11.5	108
318	Unveiling Electronic Properties in Metal-Phthalocyanine-Based Pyrazine-Linked Conjugated Two-Dimensional Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 16810-16816	16.4	107
317	Tandem intercalation strategy for single-layer nanosheets as an effective alternative to conventional exfoliation processes. <i>Nature Communications</i> , <b>2015</b> , 6, 5763	17.4	106
316	Quantum spin Hall effect and topological phase transition in two-dimensional square transition-metal dichalcogenides. <i>Physical Review B</i> , <b>2015</b> , 92,	3.3	106
315	Unravelling phenomenon of internal rotation in B13+ through chemical bonding analysis. <i>Chemical Communications</i> , <b>2011</b> , 47, 6242-4	5.8	106
314	On the reticular construction concept of covalent organic frameworks. <i>Beilstein Journal of Nanotechnology</i> , <b>2010</b> , 1, 60-70	3	106
313	Defects in MOFs: a thorough characterization. <i>ChemPhysChem</i> , <b>2012</b> , 13, 2025-9	3.2	105
312	Control of biaxial strain in single-layer molybdenite using local thermal expansion of the substrate. <i>2D Materials</i> , <b>2015</b> , 2, 015006	5.9	104

311	Sigma and pi contributions to the induced magnetic field: indicators for the mobility of electrons in molecules. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 302-9	3.5	103
310	Precise and reversible band gap tuning in single-layer MoSe <sub>2</sub> by uniaxial strain. <i>Nanoscale</i> , <b>2016</b> , 8, 2589-93	9.3	102
309	Fabrication of highly uniform gel coatings by the conversion of surface-anchored metal-organic frameworks. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 8-11	16.4	102
308	Highly effective hydrogen isotope separation in nanoporous metal-organic frameworks with open metal sites: direct measurement and theoretical analysis. <i>ACS Nano</i> , <b>2014</b> , 8, 761-70	16.7	101
307	B18(2-): a quasi-planar bowl member of the Wankel motor family. <i>Chemical Communications</i> , <b>2014</b> , 50, 8140-3	5.8	98
306	Sigma-antiaromaticity in cyclobutane, cubane, and other molecules with saturated four-membered rings. <i>Organic Letters</i> , <b>2003</b> , 5, 23-6	6.2	94
305	Study of angiotensin-(1-7) vasoactive peptide and its beta-cyclodextrin inclusion complexes: complete sequence-specific NMR assignments and structural studies. <i>Peptides</i> , <b>2007</b> , 28, 2199-210	3.8	93
304	DFTB Parameters for the Periodic Table: Part 1, Electronic Structure. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 4006-17	6.4	91
303	Theoretical studies on the smallest fullerene: from monomer to oligomers and solid States. <i>Chemistry - A European Journal</i> , <b>2004</b> , 10, 963-70	4.8	87
302	Evaluation of aromaticity: A new dissected NICS model based on canonical orbitals. <i>Physical Chemistry Chemical Physics</i> , <b>2003</b> , 5, 246-251	3.6	86
301	Transition-metal dichalcogenide bilayers: Switching materials for spintronic and valleytronic applications. <i>Physical Review B</i> , <b>2014</b> , 90,	3.3	85
300	Hydrogen sieving and storage in fullerene intercalated graphite. <i>Nano Letters</i> , <b>2007</b> , 7, 1-5	11.5	85
299	C36, a hexavalent building block for fullerene compounds and solids. <i>Chemical Physics Letters</i> , <b>1999</b> , 300, 369-378	2.5	85
298	Spontaneous ripple formation in MoS <sub>2</sub> monolayers: electronic structure and transport effects. <i>Advanced Materials</i> , <b>2013</b> , 25, 5473-5	24	83
297	Ca <sub>4</sub> Be and Ca <sub>3</sub> Be <sub>2</sub> (-): global minima with a planar pentacoordinate carbon atom. <i>Chemical Communications</i> , <b>2010</b> , 46, 8776-8	5.8	83
296	Highly Sensitive Electromechanical Piezoresistive Pressure Sensors Based on Large-Area Layered PtSe Films. <i>Nano Letters</i> , <b>2018</b> , 18, 3738-3745	11.5	82
295	Correction for dispersion and Coulombic interactions in molecular clusters with density functional derived methods: application to polycyclic aromatic hydrocarbon clusters. <i>Journal of Chemical Physics</i> , <b>2009</b> , 130, 244304	3.9	81
294	Antiaromaticity in bare deltahedral silicon clusters satisfying Wade's and Hirsch's rules: an apparent correlation of antiaromaticity with high symmetry. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 430-1	16.4	79

293	Engineering crystalline quasi-two-dimensional polyaniline thin film with enhanced electrical and chemiresistive sensing performances. <i>Nature Communications</i> , <b>2019</b> , 10, 4225	17.4	78
292	Boron-Nitrogen analogues of the fullerenes: the isolated-square rule. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1996</b> , 92, 2197-2201		78
291	Density Functional Theory and Beyond for Band-Gap Screening: Performance for Transition-Metal Oxides and Dichalcogenides. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 2950-8	6.4	77
290	Energetics of Fullerenes with Four-Membered Rings. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 6984-6991		77
289	Noncovalent bifunctional organocatalysts: powerful tools for contiguous quaternary-tertiary stereogenic carbon formation, scope, and origin of enantioselectivity. <i>Chemistry - A European Journal</i> , <b>2012</b> , 18, 4088-98	4.8	75
288	Aromaticity of four-membered-ring 6pi-electron systems: N <sub>2</sub> S <sub>2</sub> and Li <sub>2</sub> C <sub>4</sub> H <sub>4</sub> . <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 3132-8	16.4	75
287	Polyoxometalates made of gold: the polyoxoaurate [Au(III) <sub>4</sub> As(V) <sub>4</sub> O <sub>20</sub> ] <sup>8-</sup> . <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 1886-9	16.4	74
286	Capture of heavy hydrogen isotopes in a metal-organic framework with active Cu(I) sites. <i>Nature Communications</i> , <b>2017</b> , 8, 14496	17.4	73
285	Revealing unusual chemical bonding in planar hyper-coordinate Ni <sub>2</sub> Ge and quasi-planar Ni <sub>2</sub> Si two-dimensional crystals. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 26043-8	3.6	73
284	Structure and Fluxionality of B Probed by Infrared Photodissociation Spectroscopy. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 501-504	16.4	70
283	Extension of the Universal Force Field for Metal-Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 5215-5225	6.4	70
282	Dynamical behavior of Borospherene: A Nanobubble. <i>Scientific Reports</i> , <b>2015</b> , 5, 11287	4.9	70
281	A semiconducting layered metal-organic framework magnet. <i>Nature Communications</i> , <b>2019</b> , 10, 3260	17.4	69
280	Poly(perfluoroalkylation) of metallic nitride fullerenes reveals addition-pattern guidelines: synthesis and characterization of a family of Sc <sub>3</sub> N@C <sub>80</sub> (CF <sub>3</sub> ) <sub>n</sub> (n = 2-16) and their radical anions. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 2672-90	16.4	69
279	A Single-Material Logical Junction Based on 2D Crystal PdS <sub>2</sub> . <i>Advanced Materials</i> , <b>2016</b> , 28, 853-6	24	68
278	Enhancement of Chemical Stability and Crystallinity in Porphyrin-Containing Covalent Organic Frameworks by Intramolecular Hydrogen Bonds. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 13290-13294	3.6	67
277	Post-anti-van der Hoff-Le Bel motif in atomically thin germanium-copper alloy film. <i>Physical Chemistry Chemical Physics</i> , <b>2015</b> , 17, 17545-51	3.6	65
276	Planar tetracoordinate carbons in cyclic hydrocarbons. <i>Organic Letters</i> , <b>2005</b> , 7, 1509-12	6.2	65

275	Structural and electronic properties of graphene nanoflakes. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	64
274	Two-Dimensional Boronate Ester Covalent Organic Framework Thin Films with Large Single Crystalline Domains for a Neuromorphic Memory Device. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 8218-8224	16.4	63
273	H <sub>2</sub> adsorption in metal-organic frameworks: dispersion or electrostatic interactions?. <i>Chemistry - A European Journal</i> , <b>2008</b> , 14, 6597-600	4.8	63
272	Single-Layer TlO: A Metal-Shrouded 2D Semiconductor with High Electronic Mobility. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 11694-11697	16.4	60
271	What is the maximum coordination number in a planar structure?. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 4275-6	16.4	60
270	Nanolubrication: How Do MoS <sub>2</sub> -Based Nanostructures Lubricate?. <i>Journal of Physical Chemistry C</i> , <b>2008</b> , 112, 17764-17767	3.8	58
269	Energetics of fullerenes with heptagonal rings. <i>Journal of the Chemical Society, Faraday Transactions</i> , <b>1996</b> , 92, 2203		58
268	AuToGraFS: automatic topological generator for framework structures. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 9607-14	2.8	57
267	Visualizing electronic interactions between iron and carbon by X-ray chemical imaging and spectroscopy. <i>Chemical Science</i> , <b>2015</b> , 6, 3262-3267	9.4	56
266	Structure and bonding of IrB <sub>12</sub> —converting a rigid boron B <sub>12</sub> platelet to a Wankel motor. <i>RSC Advances</i> , <b>2016</b> , 6, 27177-27182	3.7	56
265	PtTe Monolayer: Two-Dimensional Electrocatalyst with High Basal Plane Activity toward Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 12732-12735	16.4	56
264	Highly Crystalline and Semiconducting Imine-Based Two-Dimensional Polymers Enabled by Interfacial Synthesis. <i>Angewandte Chemie - International Edition</i> , <b>2020</b> , 59, 6028-6036	16.4	55
263	Identification of Prime Factors to Maximize the Photocatalytic Hydrogen Evolution of Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 9752-9762	16.4	55
262	Electronic properties of transition-metal dichalcogenides. <i>MRS Bulletin</i> , <b>2015</b> , 40, 577-584	3.2	55
261	Dynamical behavior of boron clusters. <i>Nanoscale</i> , <b>2016</b> , 8, 17639-17644	7.7	55
260	Two-Dimensional Kagome Lattices Made of Hetero Triangulenes Are Dirac Semimetals or Single-Band Semiconductors. <i>Journal of the American Chemical Society</i> , <b>2019</b> , 141, 743-747	16.4	55
259	From layers to nanotubes: Transition metal disulfides TMS <sub>2</sub> . <i>European Physical Journal B</i> , <b>2012</b> , 85, 1	1.2	54
258	A noble-metalate bowl: the polyoxo-6-vanado(V)-7-palladate(II) [Pd <sub>7</sub> V <sub>6</sub> O <sub>24</sub> (OH) <sub>2</sub> ] <sup>6-</sup> . <i>Angewandte Chemie - International Edition</i> , <b>2010</b> , 49, 7807-11	16.4	53



257	Fluxional Boron Clusters: From Theory to Reality. <i>Accounts of Chemical Research</i> , <b>2019</b> , 52, 2732-2744	24.3	52
256	Palladastannatranes $\sigma$ -PdII- $\delta$ NIV Dative Bond. <i>European Journal of Inorganic Chemistry</i> , <b>2008</b> , 2008, 4225-4229		52
255	Two-dimensional inversion-asymmetric topological insulators in functionalized III-Bi bilayers. <i>Physical Review B</i> , <b>2015</b> , 91,	3.3	51
254	$^{13}\text{C}$ NMR fingerprint characterizes long time-scale structure of Sc $_3\text{N}@$ C $_{80}$ endohedral fullerene. <i>Magnetic Resonance in Chemistry</i> , <b>2004</b> , 42 Spec no, S199-201	2.1	51
253	(NHCMe)SiCl $_4$ : a versatile carbene transfer reagent $\sigma$ -synthesis from silicochloroform. <i>Chemical Science</i> , <b>2013</b> , 4, 77-83	9.4	50
252	Room temperature quantum spin Hall states in two-dimensional crystals composed of pentagonal rings and their quantum wells. <i>NPG Asia Materials</i> , <b>2016</b> , 8, e264-e264	10.3	49
251	Structure and Electron Delocalization in Al $_4$ (2-) and Al $_4$ (4.). <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 775-81	6.4	49
250	Two-dimensional ferroelastic topological insulators in single-layer Janus transition metal dichalcogenides MSe(M=Mo,W). <i>Physical Review B</i> , <b>2018</b> , 98,	3.3	48
249	On the mechanism of hydrogen activation by frustrated Lewis pairs. <i>Chemistry - A European Journal</i> , <b>2013</b> , 19, 17413-24	4.8	48
248	Two-dimensional transition metal dichalcogenides with a hexagonal lattice: Room-temperature quantum spin Hall insulators. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	47
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