

Thomas Heine

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	A perfect match between borophene and aluminium in the ALB heterostructure with covalent Al-B bonds, multiple Dirac points and a high Fermi velocity.. <i>Chemical Science</i> , 2022 , 13, 1016-1022	9.4	1
381	Statistical Representation of Stacking Disorder in Layered Covalent Organic Frameworks. <i>Chemistry of Materials</i> , 2022 , 34, 2376-2381	9.6	2
380	Isotope-selective pore opening in a flexible metal-organic framework.. <i>Science Advances</i> , 2022 , 8, eabn7035	11.5	4
379	On-Surface Formation of Cyano-Vinylene Linked Chains by Knoevenagel Condensation. <i>Chemistry - A European Journal</i> , 2021 , 27, 17336-17340	4.8	1
378	Half-Auxeticity and Anisotropic Transport in Pd Decorated Two-Dimensional Boron Sheets. <i>Nano Letters</i> , 2021 , 21, 2356-2362	11.5	9
377	Enhancement of basal plane electrocatalytic hydrogen evolution activity via joint utilization of trivial and non-trivial surface states. <i>Applied Materials Today</i> , 2021 , 22, 100921	6.6	5
376	Chirality Remote Control in Nanoporous Materials by Circularly Polarized Light. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7059-7068	16.4	9
375	Oriented Growth of In-Oxo Chain Based Metal-Porphyrin Framework Thin Film for High-Sensitive Photodetector. <i>Advanced Science</i> , 2021 , 8, 2100548	13.6	7
374	2D Honeycomb-Kagome Polymer Tandem as Effective Metal-Free Photocatalysts for Water Splitting. <i>Advanced Materials</i> , 2021 , 33, e2008645	24	19
373	Strong Binding of Noble Gases to [BX]: A Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 4760-4765	2.8	3
372	A Two-Dimensional Polyimide-Graphene Heterostructure with Ultra-fast Interlayer Charge Transfer. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 13859-13864	16.4	2
371	A Two-Dimensional Polyimide-Graphene Heterostructure with Ultra-fast Interlayer Charge Transfer. <i>Angewandte Chemie</i> , 2021 , 133, 13978-13983	3.6	
370	Surface-Modified Phthalocyanine-Based Two-Dimensional Conjugated Metal-Organic Framework Films for Polarity-Selective Chemiresistive Sensing. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 18666-18672	16.4	12
369	Liquid Exfoliated SnP ₃ Nanosheets for Very High Areal Capacity Lithium-Ion Batteries. <i>Advanced Energy Materials</i> , 2021 , 11, 2002364	21.8	17
368	Lithium-Assisted Exfoliation of Palladium Thiophosphate Nanosheets for Photoelectrocatalytic Water Splitting. <i>ACS Applied Nano Materials</i> , 2021 , 4, 441-448	5.6	3
367	BX(H): exploring the limits of isotopologue selectivity of hydrogen adsorption.. <i>RSC Advances</i> , 2021 , 11, 28466-28475	3.7	
366	Comprehensive Bonding Analysis of Tetravalent f-Element Complexes of the Type [M(salen)]. <i>Inorganic Chemistry</i> , 2021 , 60, 2514-2525	5.1	10

365	Surface-Modified Phthalocyanine-Based Two-Dimensional Conjugated Metal-Organic Framework Films for Polarity-Selective Chemiresistive Sensing. <i>Angewandte Chemie</i> , 2021 , 133, 18814-18820	3.6	0
364	Interfacial Synthesis of Layer-Oriented 2D Conjugated Metal-Organic Framework Films toward Directional Charge Transport. <i>Journal of the American Chemical Society</i> , 2021 , 143, 13624-13632	16.4	6
363	Rational Design of Two-Dimensional Binary Polymers from Heterotriangulenes for Photocatalytic Water Splitting. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 8134-8140	6.4	6
362	Investigation of CO Orientational Dynamics through Simulated NMR Line Shapes*. <i>ChemPhysChem</i> , 2021 , 22, 2336-2341	3.2	1
361	High-Mobility Semiconducting Two-Dimensional Conjugated Covalent Organic Frameworks with π -Type Doping. <i>Journal of the American Chemical Society</i> , 2020 , 142, 21622-21627	16.4	32
360	Analytical approach to phonon calculations in the SCC-DFTB framework. <i>Journal of Chemical Physics</i> , 2020 , 153, 144109	3.9	1
359	Making 2D topological polymers a reality. <i>Nature Materials</i> , 2020 , 19, 823-824	27	12
358	London Dispersion Governs the Interaction Mechanism of Small Polar and Nonpolar Molecules in Metal-Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 11985-11989	3.8	5
357	Topological two-dimensional polymers. <i>Chemical Society Reviews</i> , 2020 , 49, 2007-2019	58.5	39
356	Small Crown-Ether Complexes as Molecular Models for Dihydrogen Adsorption in Undercoordinated Extraframework Cations in Zeolites. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 9409-9415	3.8	2
355	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> , 2020 , 59, 8218-8224	16.4	63
354	Benchmark of Simplified Time-Dependent Density Functional Theory for UV-Vis Spectral Properties of Porphyrinoids. <i>Advanced Theory and Simulations</i> , 2020 , 3, 1900192	3.5	4
353	Zweidimensionale Edelmetallchalkogenide und -phosphochalkogenide. <i>Angewandte Chemie</i> , 2020 , 132, 9328-9341	3.6	2
352	Two-Dimensional Noble-Metal Chalcogenides and Phosphochalcogenides. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 9242-9254	16.4	44
351	Artificial relativistic molecules. <i>Nature Communications</i> , 2020 , 11, 815	17.4	4
350	Two-Dimensional Boronate Ester Covalent Organic Framework Thin Films with Large Single Crystalline Domains for a Neuromorphic Memory Device. <i>Angewandte Chemie</i> , 2020 , 132, 8295-8301	3.6	18
349	Highly Crystalline and Semiconducting Imine-Based Two-Dimensional Polymers Enabled by Interfacial Synthesis. <i>Angewandte Chemie</i> , 2020 , 132, 6084-6092	3.6	12
348	Highly Crystalline and Semiconducting Imine-Based Two-Dimensional Polymers Enabled by Interfacial Synthesis. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 6028-6036	16.4	55

347	Proximity Effect in Crystalline Framework Materials: Stacking-Induced Functionality in MOFs and COFs. <i>Advanced Functional Materials</i> , 2020 , 30, 1908004	15.6	36
346	Identification of Prime Factors to Maximize the Photocatalytic Hydrogen Evolution of Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020 , 142, 9752-9762	16.4	55
345	A memory nanodevice based on Zn-MOF-74: a molecular dynamics study. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 1567-1570	7.1	4
344	¶PdBi ₂ monolayer: two-dimensional topological metal with superior catalytic activity for carbon dioxide electroreduction to formic acid. <i>Materials Today Advances</i> , 2020 , 8, 100091	7.4	7
343	Fragment-Based Restricted Active Space Configuration Interaction with Second-Order Corrections Embedded in Periodic Hartree-Fock Wave Function. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 7100-7108	6.4	7
342	Stone-Wales Defects Cause High Proton Permeability and Isotope Selectivity of Single-Layer Graphene. <i>Advanced Materials</i> , 2020 , 32, e2002442	24	14
341	Near-atomic-scale observation of grain boundaries in a layer-stacked two-dimensional polymer. <i>Science Advances</i> , 2020 , 6, eabb5976	14.3	18
340	Blue Phosphorene Bilayer Is a Two-Dimensional Metal and an Unambiguous Classification Scheme for Buckled Hexagonal Bilayers. <i>Physical Review Letters</i> , 2020 , 125, 196401	7.4	7
339	Crystal size versus paddle wheel deformability: selective gated adsorption transitions of the switchable metal-organic frameworks DUT-8(Co) and DUT-8(Ni). <i>Journal of Materials Chemistry A</i> , 2019 , 7, 21459-21475	13	34
338	Fluxional Boron Clusters: From Theory to Reality. <i>Accounts of Chemical Research</i> , 2019 , 52, 2732-2744	24.3	52
337	Unveiling Electronic Properties in Metal-Phthalocyanine-Based Pyrazine-Linked Conjugated Two-Dimensional Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2019 , 141, 16810-16816	16.4	107
336	Engineering crystalline quasi-two-dimensional polyaniline thin film with enhanced electrical and chemiresistive sensing performances. <i>Nature Communications</i> , 2019 , 10, 4225	17.4	78
335	Dissolving uptake-hindering surface defects in metal-organic frameworks. <i>Chemical Science</i> , 2019 , 10, 153-160	9.4	36
334	Conformational isomerism controls collective flexibility in metal-organic framework DUT-8(Ni). <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 674-680	3.6	27
333	Bridging the Green Gap: Metal-Organic Framework Heteromultilayers Assembled from Porphyrinic Linkers Identified by Using Computational Screening. <i>Chemistry - A European Journal</i> , 2019 , 25, 7847-7851	4.8	18
332	High-Precision Size Recognition and Separation in Synthetic 1D Nanochannels. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 15922-15927	16.4	24
331	High-Precision Size Recognition and Separation in Synthetic 1D Nanochannels. <i>Angewandte Chemie</i> , 2019 , 131, 16069-16074	3.6	9
330	A Ligand Field Molecular Mechanics Study of CO ₂ -Induced Breathing in the Metal-Organic Framework DUT-8(Ni). <i>Advanced Theory and Simulations</i> , 2019 , 2, 1900098	3.5	5

329	A semiconducting layered metal-organic framework magnet. <i>Nature Communications</i> , 2019 , 10, 3260	17.4	69
328	On the Chemistry and Diffusion of Hydrogen in the Interstitial Space of Layered Crystals h-BN, MoS ₂ , and Graphite. <i>Small</i> , 2019 , 15, e1901722	11	2
327	On-water surface synthesis of crystalline, few-layer two-dimensional polymers assisted by surfactant monolayers. <i>Nature Chemistry</i> , 2019 , 11, 994-1000	17.6	149
326	A Nitrogen-Rich 2D sp ² -Carbon-Linked Conjugated Polymer Framework as a High-Performance Cathode for Lithium-Ion Batteries. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 849-853	16.4	164
325	Non equilibrium anisotropic excitons in atomically thin ReS ₂ . <i>2D Materials</i> , 2019 , 6, 015012	5.9	18
324	Two-Dimensional Kagome Lattices Made of Hetero Triangulenes Are Dirac Semimetals or Single-Band Semiconductors. <i>Journal of the American Chemical Society</i> , 2019 , 141, 743-747	16.4	55
323	Ultrastable Imine-Based Covalent Organic Frameworks for Sulfuric Acid Recovery: An Effect of Interlayer Hydrogen Bonding. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 5797-5802	16.4	118
322	Ultrastable Imine-Based Covalent Organic Frameworks for Sulfuric Acid Recovery: An Effect of Interlayer Hydrogen Bonding. <i>Angewandte Chemie</i> , 2018 , 130, 5899-5904	3.6	34
321	Photocarrier generation from interlayer charge-transfer transitions in WS ₂ -graphene heterostructures. <i>Science Advances</i> , 2018 , 4, e1700324	14.3	115
320	Large-grain MBE-grown GaSe on GaAs with a Mexican hat-like valence band dispersion. <i>Npj 2D Materials and Applications</i> , 2018 , 2,	8.8	34
319	Conduction-band valley spin splitting in single-layer H-Tl ₂ O. <i>Physical Review B</i> , 2018 , 97,	3.3	26
318	Tuning the electronic structure of graphene through alkali metal and halogen atom intercalation. <i>Solid State Communications</i> , 2018 , 272, 22-27	1.6	6
317	Toward separation of hydrogen isotopologues by exploiting zero-point energy difference at strongly attractive adsorption site models. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25545 ²⁻¹	4	4
316	Dynamics of the OH stretching mode in crystalline Ba(ClO) ₄ BHO. <i>Journal of Chemical Physics</i> , 2018 , 148, 054307	3.9	3
315	Transport of hydrogen isotopes through interlayer spacing in van der Waals crystals. <i>Nature Nanotechnology</i> , 2018 , 13, 468-472	28.7	26
314	Two-dimensional ferroelastic topological insulators in single-layer Janus transition metal dichalcogenides MSe ₂ (M=Mo,W). <i>Physical Review B</i> , 2018 , 98,	3.3	48
313	Adsorption of water, sulfates and chloride on arsenopyrite surface. <i>Applied Surface Science</i> , 2018 , 434, 389-399	6.7	12
312	Two-dimensional Pd ₃ P ₂ S ₈ semiconductors as photocatalysts for the solar-driven oxygen evolution reaction: a theoretical investigation. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 23495-23501	13	33

311	A Nitrogen-Rich 2D sp ² -Carbon-Linked Conjugated Polymer Framework as a High-Performance Cathode for Lithium-Ion Batteries. <i>Angewandte Chemie</i> , 2018 , 131, 859	3.6	2
310	2D Crystals in Three Dimensions: Electronic Decoupling of Single-Layered Platelets in Colloidal Nanoparticles. <i>Small</i> , 2018 , 14, e1803910	11	4
309	Cavitation energies can outperform dispersion interactions. <i>Nature Chemistry</i> , 2018 , 10, 1252-1257	17.6	39
308	PtTe Monolayer: Two-Dimensional Electrocatalyst with High Basal Plane Activity toward Oxygen Reduction Reaction. <i>Journal of the American Chemical Society</i> , 2018 , 140, 12732-12735	16.4	56
307	High-mobility band-like charge transport in a semiconducting two-dimensional metal-organic framework. <i>Nature Materials</i> , 2018 , 17, 1027-1032	27	216
306	Photochemical Creation of Covalent Organic 2D Monolayer Objects in Defined Shapes via a Lithographic 2D Polymerization. <i>ACS Nano</i> , 2018 , 12, 11294-11306	16.7	13
305	Probing charge transfer characteristics in a donor-acceptor metal-organic framework by Raman spectroelectrochemistry and pressure-dependence studies. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25772-25779	3.6	19
304	Highly Sensitive Electromechanical Piezoresistive Pressure Sensors Based on Large-Area Layered PtSe Films. <i>Nano Letters</i> , 2018 , 18, 3738-3745	11.5	82
303	Nuclear quantum effects on adsorption of H ₂ and isotopologues on metal ions. <i>Chemical Physics Letters</i> , 2017 , 670, 64-70	2.5	11
302	High-Performance 2D p-Type Transistors Based on GaSe Layers: An Ab Initio Study. <i>Advanced Electronic Materials</i> , 2017 , 3, 1600399	6.4	18
301	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> , 2017 , 29, 2074-2080	9.6	188
300	GeP: A Small Indirect Band Gap 2D Crystal with High Carrier Mobility and Strong Interlayer Quantum Confinement. <i>Nano Letters</i> , 2017 , 17, 1833-1838	11.5	228
299	Zn ²⁺ -Ion Sensing by Fluorescent Schiff Base Calix[4]arene Macrocycles. <i>Chemistry - A European Journal</i> , 2017 , 23, 3824-3827	4.8	24
298	Two-Dimensional Topological Insulators: Progress and Prospects. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1905-1919	6.4	110
297	Structure and Fluxionality of B Probed by Infrared Photodissociation Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 501-504	16.4	70
296	Zweidimensionales Haeckelit-NbS ₂ – ein diamagnetischer Halbleiter mit Nb ⁴⁺ -Ionen und hoher Ladungsträgermobilität. <i>Angewandte Chemie</i> , 2017 , 129, 10348-10352	3.6	
295	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16178-16188	3.6	5
294	Covalent Co-O-V and Sb-N Bonds Enable Polyoxovanadate Charge Control. <i>Inorganic Chemistry</i> , 2017 , 56, 7120-7126	5.1	14

293	Double Dirac point semimetal in 2D material: Ta ₂ Se ₃ . <i>2D Materials</i> , 2017 , 4, 025111	5.9	14
292	Two-Dimensional Haeckelite NbS ₂ : A Diamagnetic High-Mobility Semiconductor with Nb Ions. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 10214-10218	16.4	24
291	Defect Healing and Charge Transfer-Mediated Valley Polarization in MoS ₂ /MoSe ₂ /MoS ₂ Trilayer van der Waals Heterostructures. <i>Nano Letters</i> , 2017 , 17, 4130-4136	11.5	44
290	Ionic Covalent Organic Frameworks: Design of a Charged Interface Aligned on 1D Channel Walls and Its Unusual Electrostatic Functions. <i>Angewandte Chemie</i> , 2017 , 129, 5064-5068	3.6	26
289	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> , 2017 , 56, 4982-4986	16.4	166
288	Capture of heavy hydrogen isotopes in a metal-organic framework with active Cu(I) sites. <i>Nature Communications</i> , 2017 , 8, 14496	17.4	73
287	3D Synergistically Active Carbon Nanofibers for Improved Oxygen Evolution. <i>Advanced Energy Materials</i> , 2017 , 7, 1602928	21.8	111
286	Electronic structure and oxygen reduction on tunable [Ti(IV)Pc] ₂ ⁺ and Ti(II)Pc titanyl-phthalocyanines: A quantum chemical prediction. <i>Computational Materials Science</i> , 2017 , 129, 24-36	3.2	5
285	Untersuchung der Struktur und Dynamik des B ₁₃ ⁺ mithilfe der Infrarot-Photodissoziations-spektroskopie. <i>Angewandte Chemie</i> , 2017 , 129, 515-519	3.6	15
284	Two-dimensional crystal CuS ₂ Electronic and structural properties. <i>2D Materials</i> , 2017 , 4, 015041	5.9	13
283	The effects of halogen elements on the opening of an icosahedral B framework. <i>Journal of Chemical Physics</i> , 2017 , 147, 144302	3.9	2
282	Explicit treatment of hydrogen bonds in the universal force field: Validation and application for metal-organic frameworks, hydrates, and host-guest complexes. <i>Journal of Chemical Physics</i> , 2017 , 147, 161705	3.9	9
281	Single-Layer TlO: A Metal-Shrouded 2D Semiconductor with High Electronic Mobility. <i>Journal of the American Chemical Society</i> , 2017 , 139, 11694-11697	16.4	60
280	Two-dimensional sp carbon-conjugated covalent organic frameworks. <i>Science</i> , 2017 , 357, 673-676	33.3	543
279	Ultrathin Layers of PdPX (X=S, Se): Two Dimensional Semiconductors for Photocatalytic Water Splitting. <i>Chemistry - A European Journal</i> , 2017 , 23, 13612-13616	4.8	44
278	Raman spectroscopy studies of the terahertz vibrational modes of a DUT-8 (Ni) metal-organic framework. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 32099-32104	3.6	35
277	Oxidation Mechanism of Arsenopyrite in the Presence of Water. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 26887-26894	3.8	6
276	Extension of the Universal Force Field for Metal-Organic Frameworks. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 5215-5225	6.4	70

275	Group 10-group 14 metal complexes [E-TM](IV): the role of the group 14 site as an L, X and Z-type ligand. <i>Dalton Transactions</i> , 2016 , 45, 14252-64	4.3	13
274	Highly oriented MOF thin film-based electrocatalytic device for the reduction of CO ₂ to CO exhibiting high faradaic efficiency. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 15320-15326	13	121
273	Two-dimensional transition metal dichalcogenides with a hexagonal lattice: Room-temperature quantum spin Hall insulators. <i>Physical Review B</i> , 2016 , 93,	3.3	47
272	Raman spectroscopy of intercalated and misfit layer nanotubes. <i>Physical Review B</i> , 2016 , 94,	3.3	8
271	Chiral Dodecanuclear Palladium(II) Thio Cluster: Synthesis, Structure, and Formation Mechanism Explored by ESI-MS and DFT Calculations. <i>Inorganic Chemistry</i> , 2016 , 55, 7811-3	5.1	2
270	Two-dimensional topological insulators in group-11 chalcogenide compounds: M ₂ Te(M=Cu,Ag). <i>Physical Review B</i> , 2016 , 93,	3.3	26
269	Proposed two-dimensional topological insulator in SiTe. <i>Physical Review B</i> , 2016 , 94,	3.3	36
268	Continuous-Wave Single-Crystal Electron Paramagnetic Resonance of Adsorption of Gases to Cupric Ions in the Zn(II)-Doped Porous Coordination Polymer Cu ₂ .965Zn _{0.035} (btc) ₂ . <i>Journal of Physical Chemistry C</i> , 2016 , 120, 27399-27411	3.8	10
267	Multiple-component covalent organic frameworks. <i>Nature Communications</i> , 2016 , 7, 12325	17.4	147
266	Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation. <i>Angewandte Chemie</i> , 2016 , 128, 7937-7941	3.6	28
265	Platinum-Containing Polyoxometalates: syn- and anti-[Pt(II) ₂ (PW ₁₁ O ₃₉) ₂](10-) and Formation of the Metal-Metal-Bonded di-Pt(III) Derivatives. <i>Chemistry - A European Journal</i> , 2016 , 22, 5514-9	4.8	15
264	Density-functional-based tight-binding parameterization of Mo, C, H, O and Si for studying hydrogenation reactions on molybdenum carbide. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	2
263	Room temperature quantum spin Hall states in two-dimensional crystals composed of pentagonal rings and their quantum wells. <i>NPG Asia Materials</i> , 2016 , 8, e264-e264	10.3	49
262	Effect of compression on the electronic, optical and transport properties of MoS ₂ /graphene-based junctions. <i>2D Materials</i> , 2016 , 3, 025018	5.9	32
261	The importance of dynamics studies on the design of sandwich structures: a CrB ₂₄ case. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 18336-41	3.6	5
260	Stacking dependence of carrier transport properties in multilayered black phosphorous. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 075001	1.8	12
259	Prediction of topological phase transition in X ₂ -SiGe monolayers. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3669-74	3.6	11
258	Precise and reversible band gap tuning in single-layer MoSe ₂ by uniaxial strain. <i>Nanoscale</i> , 2016 , 8, 2589-93	9.3	102

257	Self-assembly of endohedral metallofullerenes: a decisive role of cooling gas and metal-carbon bonding. <i>Nanoscale</i> , 2016 , 8, 3796-808	7.7	20
256	Controlling embedment and surface chemistry of nanoclusters in metal-organic frameworks. <i>Chemical Communications</i> , 2016 , 52, 5175-8	5.8	14
255	Rotational Isomerism, Electronic Structures, and Basicity Properties of "Fully-Reduced" V14-type Heteropolyoxovanadates. <i>Inorganic Chemistry</i> , 2016 , 55, 3777-88	5.1	16
254	Interplaying Intrinsic and Extrinsic Proton Conductivities in Covalent Organic Frameworks. <i>Chemistry of Materials</i> , 2016 , 28, 1489-1494	9.6	211
253	Mixed Matrix Membranes (MMMs) Comprising Exfoliated 2D Covalent Organic Frameworks (COFs) for Efficient CO ₂ Separation. <i>Chemistry of Materials</i> , 2016 , 28, 1277-1285	9.6	404
252	A kinetic study on the reduction of CO ₂ by frustrated Lewis pairs: from understanding to rational design. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 3567-74	3.6	28
251	The polyoxo-22-palladate(ii), [Na ₂ PdO ₁₂ (As(V)O ₄) ₁₅ (As(V)O ₃ OH)](25-). <i>Dalton Transactions</i> , 2016 , 45, 2394-8	4.3	14
250	Exploring host-guest complexation mechanisms by a molecular dynamics/quantum mechanics/continuum solvent model approach. <i>Chemical Physics Letters</i> , 2016 , 648, 170-177	2.5	6
249	Structure and bonding of IrB ₁₂ converting a rigid boron B ₁₂ platelet to a Wankel motor. <i>RSC Advances</i> , 2016 , 6, 27177-27182	3.7	56
248	On the Stability and Electronic Structure of Transition-Metal Dichalcogenide Monolayer Alloys Mo _{1-x} W _x S ₂ with X = W, Nb. <i>Electronics (Switzerland)</i> , 2016 , 5, 1	2.6	32
247	A Single-Material Logical Junction Based on 2D Crystal PdS ₂ . <i>Advanced Materials</i> , 2016 , 28, 853-6	24	68
246	Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 7806-10	16.4	121
245	Vibrationally resolved UV/Vis spectroscopy with time-dependent density functional based tight binding. <i>Journal of Chemical Physics</i> , 2016 , 145, 184102	3.9	10
244	Tight-binding approximations to time-dependent density functional theory - A fast approach for the calculation of electronically excited states. <i>Journal of Chemical Physics</i> , 2016 , 144, 184103	3.9	28
243	Spin polarization in SCC-DFTB. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	7
242	Mit variablem Abstand gestapelte lineare Ketten magnetischer Ionen: ferromagnetische Ordnung mit einer Curie-Temperatur von \approx 20 K. <i>Angewandte Chemie</i> , 2016 , 128, 12874-12879	3.6	
241	Ni on the CeO ₂ (110) and (100) surfaces: adsorption vs. substitution effects on the electronic and geometric structures and oxygen vacancies. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 11139-49	3.6	27
240	Variable van der Waals Radii Derived From a Hybrid Gaussian Charge Distribution Model for Continuum-Solvent Electrostatic Calculations. <i>Zeitschrift Fur Physikalische Chemie</i> , 2016 , 230,	3.1	1

- 239 Highly Emissive Covalent Organic Frameworks. *Journal of the American Chemical Society*, **2016**, 138, 5797-800 373
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- 237 Dynamical behavior of boron clusters. *Nanoscale*, **2016**, 8, 17639-17644 7.7 55
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