Xiao Cheng Zeng

List of Publications by Citations

620 papers	36,187 citations	94 h-index	159 g-index
645 ext. papers	40,985 ext. citations	9.1 avg, IF	7.91 L-index

#	Paper	IF	Citations
620	Defect passivation in hybrid perovskite solar cells using quaternary ammonium halide anions and cations. *Nature Energy*, **2017**, 2,	62.3	1241
619	Formation of ordered ice nanotubes inside carbon nanotubes. *Nature*, **2001**, 412, 802-5	50.4	915
618	A universal principle for a rational design of single-atom electrocatalysts. *Nature Catalysis*, **2018**, 1, 339-348	36.5	739
617	Bilayer Phosphorene: Effect of Stacking Order on Bandgap and Its Potential Applications in Thin-Film Solar Cells. *Journal of Physical Chemistry Letters*, **2014**, 5, 1289-93	6.4	659
616	Two-dimensional boron monolayer sheets. *ACS Nano*, **2012**, 6, 7443-53	16.7	548
615	High-gain and low-driving-voltage photodetectors based on organolead triiodide perovskites. *Advanced Materials*, **2015**, 27, 1912-8	24	491
614	Phosphorene Nanoribbons, Phosphorus Nanotubes, and van der Waals Multilayers. *Journal of Physical Chemistry C*, **2014**, 118, 14051-14059	3.8	467
613	Conjugated Lewis Base: Efficient Trap-Passivation and Charge-Extraction for Hybrid Perovskite Solar Cells. *Advanced Materials*, **2017**, 29, 1604545	24	431
612	Planar-to-tubular structural transition in boron clusters: B20 as the embryo of single-walled boron nanotubes. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 961-4	11.5	428
611	A droplet-based electricity generator with high instantaneous power density. *Nature*, **2020**, 578, 392-396	50.4	391
610	Tailoring Passivation Molecular Structures for Extremely Small Open-Circuit Voltage Loss in Perovskite Solar Cells. *Journal of the American Chemical Society*, **2019**, 141, 5781-5787	16.4	368
609	Strain-dependent electronic and magnetic properties of MoS2 monolayer, bilayer, nanoribbons and nanotubes. *Physical Chemistry Chemical Physics*, **2012**, 14, 13035-40	3.6	358
608	Intrinsic Ferroelasticity and/or Multiferroicity in Two-Dimensional Phosphorene and Phosphorene Analogues. *Nano Letters*, **2016**, 16, 3236-41	11.5	350
607	Evidence of hollow golden cages. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 8326-30	11.5	345
606	Coexistence and transition between Cassie and Wenzel state on pillared hydrophobic surface. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 8435-40	11.5	341
605	Simultaneously Dual Modification of Ni-Rich Layered Oxide Cathode for High-Energy Lithium-Ion Batteries. *Advanced Functional Materials*, **2019**, 29, 1808825	15.6	287
604	First-order transition in confined water between high-density liquid and low-density amorphous phases. *Nature*, **2000**, 408, 564-7	50.4	286

603	Highly stable and efficient all-inorganic lead-free perovskite solar cells with native-oxide passivation. *Nature Communications*, **2019**, 10, 16	17.4	283
602	MoS2/MX2 heterobilayers: bandgap engineering via tensile strain or external electrical field. *Nanoscale*, **2014**, 6, 2879-86	7.7	275
601	Structural prediction of thiolate-protected Au38: a face-fused bi-icosahedral Au core. *Journal of the American Chemical Society*, **2008**, 130, 7830-2	16.4	261
600	Cesium Titanium(IV) Bromide Thin Films Based Stable Lead-free Perovskite Solar Cells. *Joule*, **2018**, 2, 558-570	27.8	260
599	Metallic Nickel Hydroxide Nanosheets Give Superior Electrocatalytic Oxidation of Urea for Fuel Cells. *Angewandte Chemie - International Edition*, **2016**, 55, 12465-9	16.4	253
598	Nanosheet Supported Single-Metal Atom Bifunctional Catalyst for Overall Water Splitting. *Nano Letters*, **2017**, 17, 5133-5139	11.5	253
597	Nine new phosphorene polymorphs with non-honeycomb structures: a much extended family. *Nano Letters*, **2015**, 15, 3557-62	11.5	247
596	Adsorption of O2, H2, CO, NH3, and NO2 on ZnO Nanotube: A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2008**, 112, 5747-5755	3.8	240
595	Free-Standing Two-Dimensional Ru Nanosheets with High Activity toward Water Splitting. *ACS Catalysis*, **2016**, 6, 1487-1492	13.1	217
594	Semimetallic molybdenum disulfide ultrathin nanosheets as an efficient electrocatalyst for hydrogen evolution. *Nanoscale*, **2014**, 6, 8359-67	7.7	216
593	Investigating the structural evolution of thiolate protected gold clusters from first-principles. *Nanoscale*, **2012**, 4, 4054-72	7.7	205
592	Wetting and interfacial properties of water nanodroplets in contact with graphene and monolayer boron-nitride sheets. *ACS Nano*, **2012**, 6, 2401-9	16.7	193
591	Earth-Abundant Nontoxic Titanium(IV)-based Vacancy-Ordered Double Perovskite Halides with Tunable 1.0 to 1.8 eV Bandgaps for Photovoltaic Applications. *ACS Energy Letters*, **2018**, 3, 297-304	20.1	192
590	Freezing of Confined Water: A Bilayer Ice Phase in Hydrophobic Nanopores. *Physical Review Letters*, **1997**, 79, 5262-5265	7.4	192
589	On the phase diagram of water with density functional theory potentials: The melting temperature of ice I(h) with the Perdew-Burke-Ernzerhof and Becke-Lee-Yang-Parr functionals. *Journal of Chemical Physics*, **2009**, 130, 221102	3.9	190
588	Markedly Enhanced Oxygen Reduction Activity of Single-Atom Fe Catalysts via Integration with Fe Nanoclusters. *ACS Nano*, **2019**, 13, 11853-11862	16.7	189
587	Titanium trisulfide monolayer: theoretical prediction of a new direct-gap semiconductor with high and anisotropic carrier mobility. *Angewandte Chemie - International Edition*, **2015**, 54, 7572-6	16.4	189
586	Exploration of High-Performance Single-Atom Catalysts on Support M1/FeOx for CO Oxidation via Computational Study. *ACS Catalysis*, **2015**, 5, 544-552	13.1	179

585	A theoretical study of single-atom catalysis of CO oxidation using Au embedded 2D h-BN monolayer: a CO-promoted O2 activation. *Scientific Reports*, **2014**, 4, 5441	4.9	177
584	Tuning Electronic and Magnetic Properties of Early Transition-Metal Dichalcogenides via Tensile Strain. *Journal of Physical Chemistry C*, **2014**, 118, 7242-7249	3.8	171
583	Suppressed Ion Migration along the In-Plane Direction in Layered Perovskites. *ACS Energy Letters*, **2018**, 3, 684-688	20.1	166
582	Mechanistic Origin of the High Performance of Yolk@Shell BiS@N-Doped Carbon Nanowire Electrodes. *ACS Nano*, **2018**, 12, 12597-12611	16.7	166
581	Catalytic activities of subnanometer gold clusters (Au–Au, Au, and Au–Au) for CO oxidation. *ACS Nano*, **2011**, 5, 7818-29	16.7	163
580	Heterojunction-Depleted Lead-Free Perovskite Solar Cells with Coarse-Grained B-γ-CsSnI3 Thin Films. *Advanced Energy Materials*, **2016**, 6, 1601130	21.8	162
579	CO self-promoting oxidation on nanosized gold clusters: triangular Au3 active site and CO induced O-O scission. *Journal of the American Chemical Society*, **2013**, 135, 2583-95	16.4	162
578	Thiolate-protected Au20(SR)16 cluster: prolate Au8 core with new [Au3(SR)4] staple motif. *Journal of the American Chemical Society*, **2009**, 131, 13619-21	16.4	154
577	Mechanistic Study of the Persistent Luminescence of CaAl2O4:Eu,Nd. *Chemistry of Materials*, **2015**, 27, 2195-2202	9.6	153
576	A New Class of Folding Oligomers: Crescent Oligoamides. *Journal of the American Chemical Society*, **2000**, 122, 4219-4220	16.4	153
575	Chemical functionalization of boron-nitride nanotubes with NH3 and amino functional groups. *Journal of the American Chemical Society*, **2006**, 128, 12001-6	16.4	152
574	. *Journal of Physical Chemistry C*, **2012**, 116, 11336-11342	3.8	150
573	Multiwalled ice helixes and ice nanotubes. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 19664-7	11.5	150
572	Structures and stabilities of small silicon clusters: Ab initio molecular-orbital calculations of Si7–Si11. *Journal of Chemical Physics*, **2003**, 118, 3558-3570	3.9	149
571	Lead-Free Mixed Tin and Germanium Perovskites for Photovoltaic Application. *Journal of the American Chemical Society*, **2017**, 139, 8038-8043	16.4	148
570	Bismuth Oxychalcogenides: A New Class of Ferroelectric/Ferroelastic Materials with Ultra High Mobility. *Nano Letters*, **2017**, 17, 6309-6314	11.5	139
569	Self-assembling subnanometer pores with unusual mass-transport properties. *Nature Communications*, **2012**, 3, 949	17.4	139
568	High-Level Ab Initio Electronic Structure Calculations of Water Clusters (H2O)16 and (H2O)17: A New Global Minimum for (H2O)16. *Journal of Physical Chemistry Letters*, **2010**, 1, 3122-3127	6.4	139

567	Long-range ordered carbon clusters: a crystalline material with amorphous building blocks. *Science*, **2012**, 337, 825-8	33.3	137
566	Detection of novel gaseous states at the highly oriented pyrolytic graphite-water interface. *Langmuir*, **2007**, 23, 1778-83	4	137
565	Intrinsic electronic and transport properties of graphyne sheets and nanoribbons. *Nanoscale*, **2013**, 5, 9264-76	7.7	134
564	B2C graphene, nanotubes, and nanoribbons. *Nano Letters*, **2009**, 9, 1577-82	11.5	133
563	A Near-Infrared-Emissive Alkynyl-Protected Au24 Nanocluster. *Angewandte Chemie - International Edition*, **2015**, 54, 9683-6	16.4	130
562	Creating nanocavities of tunable sizes: hollow helices. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 11583-8	11.5	130
561	Unraveling the mechanisms of O2 activation by size-selected gold clusters: transition from superoxo to peroxo chemisorption. *Journal of the American Chemical Society*, **2012**, 134, 9438-45	16.4	129
560	CO2 Capture on h-BN Sheet with High Selectivity Controlled by External Electric Field. *Journal of Physical Chemistry C*, **2015**, 119, 6912-6917	3.8	127
559	Toward Eco-friendly and Stable Perovskite Materials for Photovoltaics. *Joule*, **2018**, 2, 1231-1241	27.8	126
558	Gold-caged metal clusters with large HOMO-LUMO gap and high electron affinity. *Journal of the American Chemical Society*, **2005**, 127, 15680-1	16.4	125
557	Endohedral silicon fullerenes sinN (27 Journal of the American Chemical Society, **2004**, 126, 13845-9	16.4	125
556	Continuous Grain-Boundary Functionalization for High-Efficiency Perovskite Solar Cells with Exceptional Stability. *CheM*, **2018**, 4, 1404-1415	16.2	124
555	Structures and relative stability of neutral gold clusters: Aun (n=15-19). *Journal of Chemical Physics*, **2006**, 125, 154303	3.9	123
554	Measurement of contact-angle hysteresis for droplets on nanopillared surface and in the Cassie and Wenzel states: a molecular dynamics simulation study. *ACS Nano*, **2011**, 5, 6834-42	16.7	121
553	Planar pentacoordinate carbon in CAl5(+): a global minimum. *Journal of the American Chemical Society*, **2008**, 130, 10394-400	16.4	120
552	Controlling Catalytic Properties of Pd Nanoclusters through Their Chemical Environment at the Atomic Level Using Isoreticular Metal□Organic Frameworks. *ACS Catalysis*, **2016**, 6, 3461-3468	13.1	120
551	Type-I van der Waals heterostructure formed by MoS and ReS monolayers. *Nanoscale Horizons*, **2017**, 2, 31-36	10.8	118
550	Interlocked catenane-like structure predicted in Au24(SR)20: implication to structural evolution of thiolated gold clusters from homoleptic gold(I) thiolates to core-stacked nanoparticles. *Journal of the American Chemical Society*, **2012**, 134, 3015-24	16.4	117

549	Metallic single-walled silicon nanotubes. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 2664-8	11.5	116
548	Structures and stability of medium silicon clusters. II. Ab initio molecular orbital calculations of Si12-Si20. *Journal of Chemical Physics*, **2004**, 120, 8985-95	3.9	116
547	Validity of Tolman's equation: How large should a droplet be?. *Journal of Chemical Physics*, **1998**, 109, 4063-4070	3.9	115
546	CO oxidation on TiO(2) (110) supported subnanometer gold clusters: size and shape effects. *Journal of the American Chemical Society*, **2013**, 135, 19336-46	16.4	113
545	Probing the structural evolution of medium-sized gold clusters: Au(n)(-) (n = 27-35). *Journal of the American Chemical Society*, **2010**, 132, 6596-605	16.4	111
544	Efficient kinetic macrocyclization. *Journal of the American Chemical Society*, **2009**, 131, 2629-37	16.4	111
543	CO oxidation catalyzed by single-walled helical gold nanotube. *Nano Letters*, **2008**, 8, 195-202	11.5	110
542	Tunable Optical Properties and Charge Separation in CH3NH3Sn(x)Pb(1-x)I3/TiO2-Based Planar Perovskites Cells. *Journal of the American Chemical Society*, **2015**, 137, 8227-36	16.4	109
541	Band-gap engineering via tailored line defects in boron-nitride nanoribbons, sheets, and nanotubes. *ACS Nano*, **2012**, 6, 4104-12	16.7	108
540	Thermal conductivity of a two-dimensional phosphorene sheet: a comparative study with graphene. *Nanoscale*, **2015**, 7, 18716-24	7.7	107
539	Icosahedral crown gold nanocluster au(43)cu(12) with high catalytic activity. *Nano Letters*, **2010**, 10, 1055-62	11.5	107
538	Motif transition in growth patterns of small to medium-sized silicon clusters. *Angewandte Chemie - International Edition*, **2005**, 44, 1491-4	16.4	107
537	Doping golden buckyballs:Cu@Au16- and Cu@Au17- cluster anions. *Angewandte Chemie - International Edition*, **2007**, 46, 2915-8	16.4	106
536	A grand unified model for liganded gold clusters. *Nature Communications*, **2016**, 7, 13574	17.4	106
535	Adsorption and Surface Reactivity on Single-Walled Boron Nitride Nanotubes Containing Stone–Wales Defects. *Journal of Physical Chemistry C*, **2007**, 111, 14105-14112	3.8	104
534	Polymorphism and polyamorphism in bilayer water confined to slit nanopore under high pressure. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 21240-5	11.5	103
533	Hydrogen Storage in Pillared Li-Dispersed Boron Carbide Nanotubes. *Journal of Physical Chemistry C*, **2008**, 112, 8458-8463	3.8	102
532	Structural transition of gold nanoclusters: from the golden cage to the golden pyramid. *ACS Nano*, **2009**, 3, 1225-30	16.7	99

531	Periodic graphene nanobuds. *Nano Letters*, **2009**, 9, 250-6	11.5	98
530	Au34-: A Fluxional Core□Shell Cluster. *Journal of Physical Chemistry C*, **2007**, 111, 8228-8232	3.8	98
529	Exploration of Half Metallicity in Edge-Modified Graphene Nanoribbons. *Journal of Physical Chemistry C*, **2010**, 114, 3937-3944	3.8	97
528	Quantized water transport: ideal desalination through graphyne-4 membrane. *Scientific Reports*, **2013**, 3, 3163	4.9	95
527	Half-Metallicity in Hybrid Graphene/Boron Nitride Nanoribbons with Dihydrogenated Edges. *Journal of Physical Chemistry C*, **2011**, 115, 9442-9450	3.8	94
526	Self-Assembly and Properties of Nonmetalated Tetraphenyl-Porphyrin on Metal Substrates. *Journal of Physical Chemistry C*, **2010**, 114, 9408-9415	3.8	94
525	Materials design of half-metallic graphene and graphene nanoribbons. *Applied Physics Letters*, **2009** , 94, 223111	3.4	93
524	Au42: an alternative icosahedral golden fullerene cage. *Journal of the American Chemical Society*, **2005**, 127, 3698-9	16.4	93
523	Stable three-center hydrogen bonding in a partially rigidified structure. *Chemistry - A European Journal*, **2001**, 7, 4352-7	4.8	93
522	van der Waals trilayers and superlattices: modification of electronic structures of MoS2 by intercalation. *Nanoscale*, **2014**, 6, 4566-71	7.7	92
521	Transition from one-dimensional water to ferroelectric ice within a supramolecular architecture. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 3481-6	11.5	89
520	Probing the planar tetra-, penta-, and hexacoordinate carbon in carbon-boron mixed clusters. *Journal of the American Chemical Society*, **2008**, 130, 2580-92	16.4	88
519	Nanoscale hydrophobic interaction and nanobubble nucleation. *Physical Review Letters*, **2004**, 93, 185701	7.4	88
518	Transition-Metal Dihydride Monolayers: A New Family of Two-Dimensional Ferromagnetic Materials with Intrinsic Room-Temperature Half-Metallicity. *Journal of Physical Chemistry Letters*, **2018**, 9, 4260-4266	6.4	87
517	Structural evolution of doped gold clusters: MAu(x)(-) (M = Si, Ge, Sn; x = 5-8). *Journal of the American Chemical Society*, **2009**, 131, 3396-404	16.4	87
516	Doping the golden cage Au16(-) with Si, Ge, and Sn. *Journal of the American Chemical Society*, **2007**, 129, 15136-7	16.4	87
515	The Tolman length: is it positive or negative?. *Journal of the American Chemical Society*, **2005**, 127, 15346-7	16.4	86
514	Relative stability of planar versus double-ring tubular isomers of neutral and anionic boron cluster B20 and B20-. *Journal of Chemical Physics*, **2006**, 124, 154310	3.9	86

513	The melting temperature of proton-disordered hexagonal ice: A computer simulation of 4-site transferable intermolecular potential model of water. *Journal of Chemical Physics*, **2000**, 112, 8534-8538	3.9	86
512	Highly confined water: two-dimensional ice, amorphous ice, and clathrate hydrates. *Accounts of Chemical Research*, **2014**, 47, 2505-13	24.3	85
511	Structural Transitions from Pyramidal to Fused Planar to Tubular to Core/Shell Compact in Gold Clusters: Aun- (n = 21□5). *Journal of Physical Chemistry C*, **2007**, 111, 4190-4198	3.8	85
510	New Mechanistic Pathways for Criegee-Water Chemistry at the Air/Water Interface. *Journal of the American Chemical Society*, **2016**, 138, 11164-9	16.4	85
509	Perovskite Chalcogenides with Optimal Bandgap and Desired Optical Absorption for Photovoltaic Devices. *Advanced Energy Materials*, **2017**, 7, 1700216	21.8	84
508	Strong aggregation and directional assembly of aromatic oligoamide macrocycles. *Journal of the American Chemical Society*, **2011**, 133, 18590-3	16.4	84
507	Self-assembly of surfactants and polymorphic transition in nanotubes. *Journal of the American Chemical Society*, **2008**, 130, 7916-20	16.4	84
506	Ferroelectricity in Covalently functionalized Two-dimensional Materials: Integration of High-mobility Semiconductors and Nonvolatile Memory. *Nano Letters*, **2016**, 16, 7309-7315	11.5	83
505	First-principles study of methane dehydrogenation on a bimetallic Cu/Ni(111) surface. *Journal of Chemical Physics*, **2009**, 131, 174702	3.9	83
504	Metal-organic Kagome lattices M3(2,3,6,7,10,11-hexaiminotriphenylene)2 (M = Ni and Cu): from semiconducting to metallic by metal substitution. *Physical Chemistry Chemical Physics*, **2015**, 17, 5954-8	3.6	82
503	Icosahedral B12-containing core-shell structures of B80. *Chemical Communications*, **2010**, 46, 3878-80	5.8	82
502	Magnetic doping of the golden cage cluster M@Au16□(M=Fe,Co,Ni). *Physical Review B*, **2009**, 79,	3.3	82
501	Guest-free monolayer clathrate and its coexistence with two-dimensional high-density ice. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 5718-22	11.5	81
500	A global search of highly stable gold-covered bimetallic clusters M@Au(n) (n=8-17): endohedral gold clusters. *ChemPhysChem*, **2006**, 7, 2275-8	3.2	80
499	Distinct ice patterns on solid surfaces with various wettabilities. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 11285-11290	11.5	79
498	Ferroelectric hexagonal and rhombic monolayer ice phases. *Chemical Science*, **2014**, 5, 1757-1764	9.4	79
497	How does water freeze inside carbon nanotubes?. *Physica A: Statistical Mechanics and Its Applications*, **2002**, 314, 462-469	3.3	79
496	Isomer identification and resolution in small gold clusters. *Journal of Chemical Physics*, **2010**, 132, 054305	3.9	78

495	Ice nanotube: What does the unit cell look like?. *Journal of Chemical Physics*, **2000**, 113, 5037	3.9	78
494	Oxidation of a two-dimensional hexagonal boron nitride monolayer: a first-principles study. *Physical Chemistry Chemical Physics*, **2012**, 14, 5545-50	3.6	77
493	Hydroxyl-decorated graphene systems as candidates for organic metal-free ferroelectrics, multiferroics, and high-performance proton battery cathode materials. *Physical Review B*, **2013**, 87,	3.3	77
492	Lowest-energy structures of water clusters (H2O)11 and (H2O)13. *Journal of Physical Chemistry A*, **2006**, 110, 11781-4	2.8	77
491	Magic-number gold nanoclusters with diameters from 1 to 3.5 nm: relative stability and catalytic activity for CO oxidation. *Nano Letters*, **2015**, 15, 682-8	11.5	76
490	Near-Barrierless Ammonium Bisulfate Formation via a Loop-Structure Promoted Proton-Transfer Mechanism on the Surface of Water. *Journal of the American Chemical Society*, **2016**, 138, 1816-9	16.4	76
489	AlxC Monolayer Sheets: Two-Dimensional Networks with Planar Tetracoordinate Carbon and Potential Applications as Donor Materials in Solar Cell. *Journal of Physical Chemistry Letters*, **2014**, 5, 2058-65	6.4	76
488	Aromatic oligoureas: enforced folding and assisted cyclization. *Organic Letters*, **2006**, 8, 803-6	6.2	76
487	Backbone-rigidified oligo(m-phenylene ethynylenes). *Journal of the American Chemical Society*, **2004**, 126, 3148-62	16.4	76
486	A new phase diagram of water under negative pressure: The rise of the lowest-density clathrate s-III. *Science Advances*, **2016**, 2, e1501010	14.3	75
485	Reversing Interfacial Catalysis of Ambipolar WSe Single Crystal. *Advanced Science*, **2020**, 7, 1901382	13.6	75
484	Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters. *Accounts of Chemical Research*, **2018**, 51, 2739-2747	24.3	75
483	Thin-Film Transformation of NH PbI to CH NH PbI Perovskite: A Methylamine-Induced Conversion-Healing Process. *Angewandte Chemie - International Edition*, **2016**, 55, 14723-14727	16.4	74
482	Planar tetracoordinate carbon strips in edge decorated graphene nanoribbon. *Journal of the American Chemical Society*, **2010**, 132, 5554-5	16.4	73
481	Ab initio study of thiolate-protected Au102 nanocluster. *ACS Nano*, **2008**, 2, 1497-503	16.7	73
480	Atomic imaging of the edge structure and growth of a two-dimensional hexagonal ice. *Nature*, **2020**, 577, 60-63	50.4	73
479	Group IVB transition metal trichalcogenides: a new class of 2D layered materials beyond graphene. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2016**, 6, 211-222	7.9	73
478	Lead-Free Dion□acobson Tin Halide Perovskites for Photovoltaics. *ACS Energy Letters*, **2019**, 4, 276-277	20.1	73

477	Monolayer and bilayer polyaniline CN: two-dimensional semiconductors with high thermal conductivity. *Nanoscale*, **2018**, 10, 4301-4310	7.7	72
476	Observation of earlier two-to-three dimensional structural transition in gold cluster anions by isoelectronic substitution: MAu(n)(-) (n=8-11; M=Ag,Cu). *Journal of Chemical Physics*, **2010**, 132, 114306	3.9	72
475	Ab initio calculation of bowl, cage, and ring isomers of C20 and C20-. *Journal of Chemical Physics*, **2005**, 122, 204109	3.9	72
474	Fabrication and understanding of CuSi-Si@carbon@graphene nanocomposites as high-performance anodes for lithium-ion batteries. *Nanoscale*, **2018**, 10, 22203-22214	7.7	72
473	CaP: A New Two-Dimensional Functional Material with Desirable Band Gap and Ultrahigh Carrier Mobility. *Journal of Physical Chemistry Letters*, **2018**, 9, 1728-1733	6.4	71
472	Fluorinating hexagonal boron nitride into diamond-like nanofilms with tunable band gap and ferromagnetism. *Journal of the American Chemical Society*, **2011**, 133, 14831-8	16.4	71
471	Two-Dimensional Single-Layer Organic–Inorganic Hybrid Perovskite Semiconductors. *Advanced Energy Materials*, **2017**, 7, 1601731	21.8	70
470	Tuning the electronic properties of monolayer and bilayer PtSe2via strain engineering. *Journal of Materials Chemistry C*, **2016**, 4, 3106-3112	7.1	70
469	Self-scrolling MoS metallic wires. *Nanoscale*, **2018**, 10, 18178-18185	7.7	70
468	Thermal Conductivity of Monolayer MoSe2 and MoS2. *Journal of Physical Chemistry C*, **2016**, 120, 26067-26075	4.8	69
467	Unusual Metallic Microporous Boron Nitride Networks. *Journal of Physical Chemistry Letters*, **2013**, 4, 3484-3488	6.4	69
466	Structural evolution of anionic silicon clusters SiN (20 . *Journal of Physical Chemistry A*, **2006**, 110, 908-12	2.8	69
465	Compression Limit of Two-Dimensional Water Constrained in Graphene Nanocapillaries. *ACS Nano*, **2015**, 9, 12197-204	16.7	68
464	Signature of coexistence of superconductivity and ferromagnetism in two-dimensional NbSe2 triggered by surface molecular adsorption. *Nature Communications*, **2016**, 7, 11210	17.4	68
463	Investigating active site of gold nanoparticle Au55(PPh3)12Cl6 in selective oxidation. *ACS Nano*, **2010**, 4, 2009-20	16.7	68
462	Insight into Chemistry on Cloud/Aerosol Water Surfaces. *Accounts of Chemical Research*, **2018**, 51, 1229-1237	24.3	67
461	Global geometry optimization of silicon clusters described by three empirical potentials. *Journal of Chemical Physics*, **2003**, 119, 1442-1450	3.9	67
460	Porous Boron Nitride with Tunable Pore Size. *Journal of Physical Chemistry Letters*, **2014**, 5, 393-8	6.4	66

459	Cooperative effects in one-dimensional chains of three-center hydrogen bonding interactions. *Journal of Chemical Physics*, **2003**, 118, 3499-3509	3.9	66
458	Edge-decorated graphene nanoribbons by scandium as hydrogen storage media. *Nanoscale*, **2012**, 4, 915-20	7.7	65
457	Mechanically robust tri-wing graphene nanoribbons with tunable electronic and magnetic properties. *Nano Letters*, **2010**, 10, 494-8	11.5	65
456	Polymorphic phases of sp3-hybridized carbon under cold compression. *Journal of the American Chemical Society*, **2012**, 134, 7530-8	16.4	64
455	Exploration of Structures of Two-Dimensional Boron-Silicon Compounds with sp(2) Silicon. *Journal of Physical Chemistry Letters*, **2013**, 4, 561-7	6.4	64
454	Formation free energy of clusters in vapor-liquid nucleation: A Monte Carlo simulation study. *Journal of Chemical Physics*, **1999**, 110, 4471-4476	3.9	64
453	Surprising Stability of Larger Criegee Intermediates on Aqueous Interfaces. *Angewandte Chemie - International Edition*, **2017**, 56, 7740-7744	16.4	63
452	Structure and stability of two dimensional phosphorene with O or NH functionalization. *RSC Advances*, **2014**, 4, 48017-48021	3.7	63
451	One-pot formation of large macrocycles with modifiable peripheries and internal cavities. *Angewandte Chemie - International Edition*, **2009**, 48, 3150-4	16.4	62
450	Melting points and thermal expansivities of proton-disordered hexagonal ice with several model potentials. *Journal of Chemical Physics*, **2004**, 121, 7926-31	3.9	62
449	Electron-Transport Properties of Few-Layer Black Phosphorus. *Journal of Physical Chemistry Letters*, **2015**, 6, 1996-2002	6.4	61
448	Stability of Metal-Encapsulating Boron Fullerene B40. *Journal of Physical Chemistry A*, **2015**, 119, 11208-14	2.8	61
447	The search for the most stable structures of silicon-carbon monolayer compounds. *Nanoscale*, **2014**, 6, 11685-91	7.7	61
446	Tuning the electronic properties of the golden buckyball by endohedral doping: M@Au16(-) (M = Ag,Zn,In). *Journal of Chemical Physics*, **2009**, 130, 051101	3.9	61
445	Lotus effect in engineered zirconia. *Nano Letters*, **2008**, 8, 988-96	11.5	61
444	Effective CO Oxidation on Endohedral Gold-Cage Nanoclusters. *Journal of Physical Chemistry C*, **2008**, 112, 8234-8238	3.8	61
443	The melting lines of model silicon calculated from coexisting solid-liquid phases. *Journal of Chemical Physics*, **2004**, 120, 1654-6	3.9	61
442	Tuning thermal contact conductance at graphene-copper interface via surface nanoengineering. *Nanoscale*, **2015**, 7, 6286-94	7.7	60

441	New Structure Model of Au22(SR)18: Bitetrahederon Golden Kernel Enclosed by [Au6(SR)6] Au(I) Complex. *Journal of Physical Chemistry Letters*, **2015**, 6, 1390-5	6.4	60
440	Argon Plasma Treatment to Tune Perovskite Surface Composition for High Efficiency Solar Cells and Fast Photodetectors. *Advanced Materials*, **2018**, 30, 1705176	24	60
439	Ferroelectric ordering in ice nanotubes confined in carbon nanotubes. *Nano Letters*, **2008**, 8, 2607-12	11.5	60
438	Highly Efficient and Anomalous Charge Transfer in van der Waals Trilayer Semiconductors. *Nano Letters*, **2017**, 17, 1623-1628	11.5	59
437	Designs of fullerene-based frameworks for hydrogen storage. *Journal of Materials Chemistry A*, **2014**, 2, 5910-5914	13	59
436	Search for Lowest-Energy Fullerenes 2: C38 to C80 and C112 to C120 *Journal of Physical Chemistry C*, **2007**, 111, 17671-17677	3.8	59
435	Search for lowest-energy fullerenes: C98 to C110. *Journal of Physical Chemistry A*, **2006**, 110, 7672-6	2.8	59
434	Stable Formamidinium-Based Perovskite Solar Cells via In Situ Grain Encapsulation. *Advanced Energy Materials*, **2018**, 8, 1800232	21.8	59
433	Two-Dimensional Metal-Free Organic Multiferroic Material for Design of Multifunctional Integrated Circuits. *Journal of Physical Chemistry Letters*, **2017**, 8, 1973-1978	6.4	58
432	Tuning the electronic properties of transition-metal trichalcogenides via tensile strain. *Nanoscale*, **2015**, 7, 15385-91	7.7	58
431	Self-Catalytic Reaction of SO and NH To Produce Sulfamic Acid and Its Implication to Atmospheric Particle Formation. *Journal of the American Chemical Society*, **2018**, 140, 11020-11028	16.4	58
430	Microscopic insight into surface wetting: relations between interfacial water structure and the underlying lattice constant. *Physical Review Letters*, **2013**, 110, 126101	7.4	58
429	Titanium Trisulfide Monolayer: Theoretical Prediction of a New Direct-Gap Semiconductor with High and Anisotropic Carrier Mobility. *Angewandte Chemie*, **2015**, 127, 7682-7686	3.6	58
428	Inorganic nanoribbons with unpassivated zigzag edges: Half metallicity and edge reconstruction. *Nano Research*, **2011**, 4, 233-239	10	58
427	Ab initio study of structural and magnetic properties of TM(n)(ferrocene)(n+1) (TM = Sc, Ti, V, Mn) sandwich clusters and nanowires (n = infinity). *ACS Nano*, **2009**, 3, 537-45	16.7	58
426	Electronic structures and electronic spectra of all-boron fullerene B40. *Chemical Communications*, **2015**, 51, 3185-8	5.8	57
425	Structures and stability of medium-sized silicon clusters. III. Reexamination of motif transition in growth pattern from Si15 to Si20. *Journal of Chemical Physics*, **2005**, 123, 164303	3.9	57
424	Ginzburg-Landau theory for the solid-liquid interface of bcc elements. *Physical Review A*, **1987**, 35, 2611-2618	2.6	57

423	Monolayer triphosphates MP (M = Sn, Ge) with excellent basal catalytic activity for hydrogen evolution reaction. *Nanoscale*, **2019**, 11, 12210-12219	7.7	56
422	Characterizing hydrophobicity of amino acid side chains in a protein environment via measuring contact angle of a water nanodroplet on planar peptide network. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 12946-12951	11.5	56
421	Unraveling the hidden function of a stabilizer in a precursor in improving hybrid perovskite film morphology for high efficiency solar cells. *Energy and Environmental Science*, **2016**, 9, 867-872	35.4	56
420	Homogenous Alloys of Formamidinium Lead Triiodide and Cesium Tin Triiodide for Efficient Ideal-Bandgap Perovskite Solar Cells. *Angewandte Chemie - International Edition*, **2017**, 56, 12658-12662	16.4	56
419	Unraveling the high-activity nature of Fe/N/C electrocatalysts for the oxygen reduction reaction: the extraordinary synergy between Fe/N4 and Fe4N. *Journal of Materials Chemistry A*, **2019**, 7, 11792-11801	13	55
418	Semiring chemistry of Au25(SR)18: fragmentation pathway and catalytic active site. *Journal of the American Chemical Society*, **2013**, 135, 18067-79	16.4	55
417	Chemically decorated boron-nitride nanoribbons. *Frontiers of Physics in China*, **2009**, 4, 367-372		55
416	Thermal stability of nanostructurally stabilized zirconium oxide. *Nanotechnology*, **2007**, 18, 415702	3.4	55
415	Possible lowest-energy geometry of silicon clusters Si21 and Si25. *Journal of the American Chemical Society*, **2003**, 125, 13318-9	16.4	55
414	Energetics and cooperativity in three-center hydrogen bonding interactions. II. Intramolecular hydrogen bonding systems. *Journal of Chemical Physics*, **2001**, 115, 6036-6041	3.9	55
413	Machine learning and artificial neural network prediction of interfacial thermal resistance between graphene and hexagonal boron nitride. *Nanoscale*, **2018**, 10, 19092-19099	7.7	55
412	SLIPS-TENG: robust triboelectric nanogenerator with optical and charge transparency using a slippery interface. *National Science Review*, **2019**, 6, 540-550	10.8	54
411	Zero-Dimensional Organic-Inorganic Perovskite Variant: Transition between Molecular and Solid Crystal. *Journal of the American Chemical Society*, **2018**, 140, 10456-10463	16.4	54
410	A photoelectron spectroscopy and ab initio study of the structures and chemical bonding of the B25(-) cluster. *Journal of Chemical Physics*, **2014**, 141, 034303	3.9	54
409	Gold-coated transition-metal anion [Mn13@Au20]- with ultrahigh magnetic moment. *Journal of the American Chemical Society*, **2007**, 129, 4110-1	16.4	54
408	Search for global minimum geometries for medium sized germanium clusters: Ge12-Ge20. *Journal of Chemical Physics*, **2005**, 122, 164305	3.9	54
407	Half-Metallic Behavior in 2D Transition Metal Dichalcogenides Nanosheets by Dual-Native-Defects Engineering. *Advanced Materials*, **2017**, 29, 1703123	24	53
406	Double metallocene nanowires. *Journal of the American Chemical Society*, **2009**, 131, 14246-8	16.4	53

405	Eighteen functional monolayer metal oxides: wide bandgap semiconductors with superior oxidation resistance and ultrahigh carrier mobility. *Nanoscale Horizons*, **2019**, 4, 592-600	10.8	51
404	Unraveling Oxygen Evolution in Li-Rich Oxides: A Unified Modeling of the Intermediate Peroxo/Superoxo-like Dimers. *Journal of the American Chemical Society*, **2019**, 141, 10751-10759	16.4	51
403	Tin and germanium based two-dimensional Ruddlesden-Popper hybrid perovskites for potential lead-free photovoltaic and photoelectronic applications. *Nanoscale*, **2018**, 10, 11314-11319	7.7	51
402	First-principles study of a carbon nanobud. *ACS Nano*, **2008**, 2, 1459-65	16.7	51
401	Structural and magnetic properties of Gd3N@C80. *Journal of Physical Chemistry B*, **2006**, 110, 23637-40	3.4	50
400	Effect of polarizability of halide anions on the ionic solvation in water clusters. *Journal of Chemical Physics*, **2003**, 119, 6083-6091	3.9	50
399	Ion-specific ice recrystallization provides a facile approach for the fabrication of porous materials. *Nature Communications*, **2017**, 8, 15154	17.4	49
398	B27(-): Appearance of the smallest planar boron cluster containing a hexagonal vacancy. *Journal of Chemical Physics*, **2015**, 142, 204305	3.9	49
397	Vapor–liquid coexistence of quasi-two-dimensional Stockmayer fluids. *Journal of Chemical Physics*, **1997**, 106, 3311-3317	3.9	49
396	Anisotropy of crystal-melt interfacial free energy of silicon by simulation. *Applied Physics Letters*, **2008**, 92, 221903	3.4	49
395	Ab initio studies of quasi-one-dimensional pentagon and hexagon ice nanotubes. *Journal of Chemical Physics*, **2003**, 118, 3913-3916	3.9	49
394	A small-system ensemble Monte Carlo simulation of supersaturated vapor: Evaluation of barrier to nucleation. *Journal of Chemical Physics*, **2000**, 112, 294-300	3.9	49
393	Double Perovskite Cs2BBiX6 (B = Ag, Cu; X = Br, Cl)/TiO2 Heterojunction: An Efficient Pb-Free Perovskite Interface for Charge Extraction. *Journal of Physical Chemistry C*, **2017**, 121, 4471-4480	3.8	48
392	Molecular dynamics simulation of supersaturated vapor nucleation in slit pore. *Journal of Chemical Physics*, **2000**, 112, 4279-4285	3.9	48
391	A vesicle cell under collision with a Janus or homogeneous nanoparticle: translocation dynamics and late-stage morphology. *Nanoscale*, **2013**, 5, 9089-100	7.7	47
390	Carrier-tunable magnetic ordering in vanadium-naphthalene sandwich nanowires. *Journal of the American Chemical Society*, **2010**, 132, 10215-7	16.4	47
389	A new strategy for folding oligo(m-phenylene ethynylenes). *Chemical Communications*, **2003**, 56-7	5.8	47
388	Large-scale molecular-dynamics simulation of nanoscale hydrophobic interaction and nanobubble formation. *Journal of Chemical Physics*, **2005**, 123, 204707	3.9	46

387	Highly efficient N fixation catalysts: transition-metal carbides MC (MXenes). *Nanoscale*, **2020**, 12, 538-547	7.7	46
386	Energetics and cooperativity in three-center hydrogen bonding interactions. I. Diacetamide-X dimers (X=HCN, CH3OH). *Journal of Chemical Physics*, **2001**, 115, 6030-6035	3.9	45
385	Water-Promoted O2 Dissociation on Small-Sized Anionic Gold Clusters. *ACS Catalysis*, **2012**, 2, 2614-2621	13.1	44
384	Structure evolution of gold cluster anions between the planar and cage structures by isoelectronic substitution: Au(n)- (n = 13-15) and MAu(n)- (n = 12-14; M = Ag, Cu). *Journal of Chemical Physics*, **2011**, 134, 054306	3.9	44
383	Graphene-like bilayer hexagonal silicon polymorph. *Nano Research*, **2010**, 3, 694-700	10	44
382	Resolving the puzzle of single-atom silver dispersion on nanosized □AlO surface for high catalytic performance. *Nature Communications*, **2020**, 11, 529	17.4	43
381	Interlayer thermal conductance within a phosphorene and graphene bilayer. *Nanoscale*, **2016**, 8, 19211-19218	7.7	43
380	Thermal contact resistance across a linear heterojunction within a hybrid graphene/hexagonal boron nitride sheet. *Physical Chemistry Chemical Physics*, **2016**, 18, 24164-70	3.6	43
379	Multiferroic materials based on organic transition-metal molecular nanowires. *Journal of the American Chemical Society*, **2012**, 134, 14423-9	16.4	42
378	Highly selective adsorption of methanol in carbon nanotubes immersed in methanol-water solution. *Journal of Chemical Physics*, **2012**, 137, 034501	3.9	42
377	Shape-persistent macrocyclic aromatic tetrasulfonamides: Molecules with nanosized cavities and their nanotubular assemblies in solid state. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 10850-5	11.5	42
376	Nucleation of water and methanol droplets on cations and anions: the sign preference. *Physical Review Letters*, **2001**, 86, 5080-3	7.4	42
375	Directly predicting limiting potentials from easily obtainable physical properties of graphene-supported single-atom electrocatalysts by machine learning. *Journal of Materials Chemistry A*, **2020**, 8, 5663-5670	13	42
374	Direct simulation evidence of generation of oxygen vacancies at the golden cage Au16 and TiO2 (110) interface for CO oxidation. *Journal of the American Chemical Society*, **2014**, 136, 15857-60	16.4	41
373	Detecting weak interactions between Au- and gas molecules: a photoelectron spectroscopic and ab initio study. *Journal of the American Chemical Society*, **2009**, 131, 9484-5	16.4	41
372	Sawtooth-like graphene nanoribbon. *Nano Research*, **2008**, 1, 40-45	10	41
371	Structural and electronic properties of Gd@C60: All-electron relativistic total-energy study. *Chemical Physics Letters*, **2006**, 425, 82-84	2.5	41
370	PtPd(111) Surface versus PtAu(111) Surface: Which One Is More Active for Methanol Oxidation?. *ACS Catalysis*, **2018**, 8, 132-143	13.1	41

369	Quasi-1D TiS Nanoribbons: Mechanical Exfoliation and Thickness-Dependent Raman Spectroscopy. *ACS Nano*, **2018**, 12, 12713-12720	16.7	41
368	Interaction of the NH2 Radical with the Surface of a Water Droplet. *Journal of the American Chemical Society*, **2015**, 137, 12070-8	16.4	40
367	Water in Inhomogeneous Nanoconfinement: Coexistence of Multilayered Liquid and Transition to Ice Nanoribbons. *ACS Nano*, **2015**, 9, 9877-84	16.7	40
366	Unraveling a generic growth pattern in structure evolution of thiolate-protected gold nanoclusters. *Nanoscale*, **2016**, 8, 7396-401	7.7	40
365	Isomerism and structural fluxionality in the Au26 and Au26(-) nanoclusters. *ACS Nano*, **2014**, 8, 7413-22	16.7	40
364	Thermodynamic expansion of nucleation free-energy barrier and size of critical nucleus near the vapor-liquid coexistence. *Journal of Chemical Physics*, **1999**, 110, 3466-3471	3.9	40
363	Unraveling structures of protection ligands on gold nanoparticle Au68(SH)32. *Science Advances*, **2015**, 1, e1400211	14.3	39
362	High-Performance Ru /CeO Single-Atom Catalyst for CO Oxidation: A Computational Exploration. *ChemPhysChem*, **2016**, 17, 3170-3175	3.2	39
361	Why Is MP2-Water "Cooler" and "Denser" than DFT-Water?. *Journal of Physical Chemistry Letters*, **2016**, 7, 680-4	6.4	39
360	Ab initio theoretical study of non-covalent adsorption of aromatic molecules on boron nitride nanotubes. *Physical Chemistry Chemical Physics*, **2011**, 13, 11766-72	3.6	39
359	Formation of HONO from the NH-promoted hydrolysis of NO dimers in the atmosphere. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 7236-7241	11.5	39
358	"Hole-" Interaction Promoted Photocatalytic Hydrodefluorination via Inner-Sphere Electron Transfer. *Journal of the American Chemical Society*, **2016**, 138, 15805-15808	16.4	38
357	Structural Evolution of Medium-Sized Gold Clusters Au(n) (n = 36, 37, 38): Appearance of Bulk-Like Face Centered Cubic Fragment. *Journal of Physical Chemistry C*, **2014**, 118, 6887-6892	3.8	38
356	Simulation Evidence of Hexagonal-to-Tetragonal ZnSe Structure Transition: A Monolayer Material with a Wide-Range Tunable Direct Bandgap. *Advanced Science*, **2015**, 2, 1500290	13.6	38
355	Hydrogen bonding and cooperative effects in mixed dimers and trimers of methanol and trifluoromethanol: An ab initio study. *Journal of Chemical Physics*, **1999**, 110, 6329-6338	3.9	38
354	Half-Metallicity in One-Dimensional Metal Trihydride Molecular Nanowires. *Journal of the American Chemical Society*, **2017**, 139, 6290-6293	16.4	37
353	Evidence of low-density and high-density liquid phases and isochore end point for water confined to carbon nanotube. *Proceedings of the National Academy of Sciences of the United States of America* , **2017**, 114, 4066-4071	11.5	37
352	Kinetic and mechanistic investigations of the direct synthesis of dimethyl carbonate from carbon dioxide over ceria nanorod catalysts. *Journal of Catalysis*, **2016**, 340, 295-301	7.3	37

351	Direct X-ray observation of trapped CO in a predesigned porphyrinic metal-organic framework. *Chemistry - A European Journal*, **2014**, 20, 7632-7	4.8	37
350	Three-dimensional network model of carbon containing only sp2-carbon bonds and boron nitride analogues. *Chemical Communications*, **2011**, 47, 4406-8	5.8	37
349	Onset of double helical structure in small-sized homoleptic gold thiolate clusters. *Journal of Physical Chemistry A*, **2009**, 113, 629-32	2.8	37
348	Aromatic oligoamide macrocycles from the bimolecular coupling of folded oligomeric precursors. *New Journal of Chemistry*, **2009**, 33, 729	3.6	37
347	Inch-Scale Grain Boundary Free Organic Crystals Developed by Nucleation Seed-Controlled Shearing Method. *ACS Applied Materials & Interfaces*, **2018**, 10, 35395-35403	9.5	37
346	Design of ferroelectric organic molecular crystals with ultrahigh polarization. *Journal of the American Chemical Society*, **2014**, 136, 6428-36	16.4	36
345	Charge-injection induced magnetism and half metallicity in single-layer hexagonal group III/V (BN, BP, AlN, AlP) systems. *Applied Physics Letters*, **2010**, 97, 093109	3.4	36
344	Self-Assembly of Janus Oligomers into Onion-like Vesicles with Layer-by-Layer Water Discharging Capability: A Minimalist Model. *ACS Nano*, **2016**, 10, 8026-37	16.7	36
343	Multifunctional Binary Monolayers Ge P : Tunable Band Gap, Ferromagnetism, and Photocatalyst for Water Splitting. *ACS Applied Materials & Interfaces*, **2018**, 10, 19897-19905	9.5	36
342	Unraveling the mechanism of selective ion transport in hydrophobic subnanometer channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 10851-6	11.5	35
341	Reaction of Criegee Intermediate with Nitric Acid at the Air-Water Interface. *Journal of the American Chemical Society*, **2018**, 140, 4913-4921	16.4	35
340	Electronic and transport properties of porous graphenes: two-dimensional benzo- and aza-fused conjugated-microporous-polymer sheets and boron nitrogen co-doped derivatives. *Journal of Materials Chemistry C*, **2014**, 2, 2902-2907	7.1	35
339	Enantioselective desymmetrization via carbonyl-directed catalytic asymmetric hydroboration and Suzuki-Miyaura cross-coupling. *Organic Letters*, **2015**, 17, 940-3	6.2	35
338	Selective directed catalytic asymmetric hydroboration of 1,1-disubstituted alkenes. *Chemical Communications*, **2012**, 48, 12180-2	5.8	35
337	Search for global-minimum geometries of medium-sized germanium clusters. II. Motif-based low-lying clusters Ge21-Ge29. *Journal of Chemical Physics*, **2006**, 124, 184309	3.9	35
336	Heterogeneous nucleation on mesoscopic wettable particles: A hybrid thermodynamic/density-functional theory. *Journal of Chemical Physics*, **2002**, 117, 1851-1868	3.9	35
335	A patching model for surface tension and the Tolman length. *Journal of Chemical Physics*, **1999**, 111, 3705-3713	3.9	35
334	Interaction of SO with the Surface of a Water Nanodroplet. *Journal of the American Chemical Society*, **2017**, 139, 17168-17174	16.4	34

333	Twisted MX/MoS heterobilayers: effect of van der Waals interaction on the electronic structure. *Nanoscale*, **2017**, 9, 19131-19138	7.7	34
332	Ab initiostudy of hydrogen adsorption on benzenoid linkers in metal□rganic framework materials. *Journal of Physics Condensed Matter*, **2007**, 19, 386220	1.8	34
331	Descriptor-Based Design Principle for Two-Dimensional Single-Atom Catalysts: Carbon Dioxide Electroreduction. *Journal of Physical Chemistry Letters*, **2020**, 11, 3481-3487	6.4	34
330	Oxygen Intercalation of Graphene on Transition Metal Substrate: An Edge-Limited Mechanism. *Journal of Physical Chemistry Letters*, **2015**, 6, 4099-105	6.4	33
329	Porphyrinic porous organic frameworks: preparation and post-synthetic modification via demetallation□emetallation. *Journal of Materials Chemistry A*, **2014**, 2, 14876-14882	13	33
328	Large negative magnetoresistance induced by anionic solid solutions in two-dimensional spin-frustrated transition metal chalcogenides. *Physical Review Letters*, **2014**, 113, 157202	7.4	33
327	Patterned Hydrogenation of Graphene: Magnetic Quantum Dot Array. *Journal of Physical Chemistry C*, **2010**, 114, 139-142	3.8	33
326	Hydrogen Production via Efficient Formic Acid Decomposition: Engineering the Surface Structure of Pd-Based Alloy Catalysts by Design. *ACS Catalysis*, **2019**, 9, 781-790	13.1	33
325	Aluminum and Nitrogen Codoped Graphene: Highly Active and Durable Electrocatalyst for Oxygen Reduction Reaction. *ACS Catalysis*, **2019**, 9, 610-619	13.1	33
324	Structural Evolution of Core-Shell Gold Nanoclusters: Au (n = 42-50). *ACS Nano*, **2016**, 10, 10013-10022	16.7	32
323	Hollow polyhedral structures in small gold-sulfide clusters. *ACS Nano*, **2011**, 5, 1441-9	16.7	32
322	Single-walled MoTe(2) nanotubes. *Nano Letters*, **2007**, 7, 2987-92	11.5	32
321	Copper(i) sulfide: a two-dimensional semiconductor with superior oxidation resistance and high carrier mobility. *Nanoscale Horizons*, **2019**, 4, 223-230	10.8	32
320	Lateral and flexural phonon thermal transport in graphene and stanene bilayers. *Physical Chemistry Chemical Physics*, **2017**, 19, 6554-6562	3.6	31
319	Nitric Acid-Amine Chemistry in the Gas Phase and at the Air-Water Interface. *Journal of the American Chemical Society*, **2018**, 140, 6456-6466	16.4	31
318	Spontaneous formation of one-dimensional hydrogen gas hydrate in carbon nanotubes. *Journal of the American Chemical Society*, **2014**, 136, 10661-8	16.4	31
317	Organometallic Hexahapto-Functionalized Graphene: Band Gap Engineering with Minute Distortion to the Planar Structure. *Journal of Physical Chemistry C*, **2013**, 117, 22156-22161	3.8	31
316	Two Dimensional Epitaxial Water Adlayer on Mica with Graphene Coating: An ab Initio Molecular Dynamics Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 3034-43	6.4	31

315	Effects of confinement on the phase behavior of supercooled water. *Chemical Physics Letters*, **1998**, 285, 278-283	2.5	31
314	Effect of uniform electric field on homogeneous vapor–liquid nucleation and phase equilibria. II. Extended simple point charge model water. *Journal of Chemical Physics*, **1999**, 110, 2533-2538	3.9	31
313	Controlling states of water droplets on nanostructured surfaces by design. *Nanoscale*, **2017**, 9, 18240-18245	7.7	30
312	Differential Permeability of Proton Isotopes through Graphene and Graphene Analogue Monolayer. *Journal of Physical Chemistry Letters*, **2016**, 7, 3395-400	6.4	30
311	Self-Assembly of Triblock Janus Nanoparticle in Nanotube. *Journal of Chemical Theory and Computation*, **2013**, 9, 179-87	6.4	30
310	CO chemisorption on the surfaces of the golden cages. *Journal of Chemical Physics*, **2009**, 131, 234305	3.9	30
309	Structures and relative stability of medium- and large-sized silicon clusters. VI. Fullerene cage motifs for low-lying clusters Si(39), Si(40), Si(50), Si(60), Si(70), and Si(80). *Journal of Chemical Physics*, **2008**, 128, 104316	3.9	30
308	Molecular dynamics of homogeneous nucleation in the vapor phase of Lennard-Jones. III. Effect of carrier gas pressure. *Journal of Chemical Physics*, **2007**, 126, 124320	3.9	30
307	A patching model for surface tension of spherical droplet and Tolman length. II. *Journal of Chemical Physics*, **1999**, 111, 10602-10610	3.9	30
306	Prediction of a new ice clathrate with record low density: A potential candidate as ice XIX in guest-free form. *Chemical Physics Letters*, **2017**, 671, 186-191	2.5	29
305	Probing Structural, Electronic, and Magnetic Properties of Iron-Doped Semiconductor Clusters $Fe_2Ge_n^-$ (n = 3–12) via Joint Photoelectron Spectroscopy and Density Functional Study. *Journal of Physical Chemistry C*, **2017**, 121, 7037-7046	3.8	29
304	The structural isomerism in gold nanoclusters. *Nanoscale*, **2018**, 10, 9476-9483	7.7	29
303	Mn monolayer modified Rh for syngas-to-ethanol conversion: a first-principles study. *Nanoscale*, **2012**, 4, 1123-9	7.7	29
302	First-principles molecular dynamics simulation of atmospherically relevant anion solvation in supercooled water droplet. *Journal of the American Chemical Society*, **2013**, 135, 15549-58	16.4	29
301	Water desalination through rim functionalized carbon nanotubes. *Journal of Materials Chemistry A*, **2019**, 7, 3583-3591	13	28
300	Computational analysis of stable hard structures in the Ti-B system. *ACS Applied Materials & Interfaces*, **2015**, 7, 15607-17	9.5	28
299	Extremely strong tubular stacking of aromatic oligoamide macrocycles. *Chemical Science*, **2015**, 6, 152-157	9.4	28
298	Graphene/antimonene/graphene heterostructure: A potential anode for sodium-ion batteries. *Carbon*, **2019**, 153, 767-775	10.4	28

297	Mechanistic Insights into Carbonyl-Directed Rhodium-Catalyzed Hydroboration: ab Initio Study of a Cyclic □Unsaturated Amide. *ACS Catalysis*, **2014**, 4, 763-773	13.1	28
296	Electronic Structures of Defective Boron Nitride Nanotubes under Transverse Electric Fields. *Journal of Physical Chemistry C*, **2008**, 112, 8424-8428	3.8	28
295	Metallic surface doping of metal halide perovskites. *Nature Communications*, **2021**, 12, 7	17.4	28
294	Criegee intermediate-hydrogen sulfide chemistry at the air/water interface. *Chemical Science*, **2017**, 8, 5385-5391	9.4	27
293	Cadmium Modified HZSM-5: A Highly Efficient Catalyst for Selective Transformation of Methanol to Aromatics. *Industrial & Engineering Chemistry Research*, **2017**, 56, 12508-12519	3.9	27
292	Molecular Dynamics Simulation of Water Nanodroplet Bounce Back from Flat and Nanopillared Surface. *Langmuir*, **2017**, 33, 10184-10192	4	27
291	Tuning the magnetic and electronic properties of bilayer graphene nanoribbons on Si(001) by bias voltage. *Physical Review B*, **2010**, 81,	3.3	27
290	Crescent oligoamides as hosts: conformation-dependent binding specificity. *Organic and Biomolecular Chemistry*, **2009**, 7, 3643-7	3.9	27
289	Freezing transition of a strongly dipolar simple fluid. *Physical Review E*, **2000**, 61, R2188-R2191	2.4	27
288	Confined water in hydrophobic nanopores: dynamics of freezing into bilayer ice. *Physical Review E*, **1999**, 60, 5833-40	2.4	27
287	Hydrogen bonding and orientation effects on the accommodation of methylamine at the air-water interface. *Journal of Chemical Physics*, **2016**, 144, 214701	3.9	27
286	Metallic Nickel Hydroxide Nanosheets Give Superior Electrocatalytic Oxidation of Urea for Fuel Cells. *Angewandte Chemie*, **2016**, 128, 12653-12657	3.6	26
285	Elastic properties of poly(vinyldene fluoride) (PVDF) crystals: A density functional theory study. *Journal of Applied Physics*, **2011**, 109, 093514	2.5	26
284	Chemisorption-Induced 2D□3D□2D Structural Transitions in Gold Heptamer: (CO)nAu7□(n = 1□4). *Journal of Physical Chemistry Letters*, **2011**, 2, 2288-2293	6.4	26
283	Homogeneous nucleation at high supersaturation and heterogeneous nucleation on microscopic wettable particles: A hybrid thermodynamic/density-functional theory. *Journal of Chemical Physics*, **2006**, 125, 144515	3.9	26
282	Design of Single-Molecule Multiferroics for Efficient Ultrahigh-Density Nonvolatile Memories. *Advanced Science*, **2019**, 6, 1801572	13.6	26
281	Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors. *ACS Catalysis*, **2018**, 8, 9702-9710	13.1	26
280	Enforced Tubular Assembly of Electronically Different Hexakis(m-Phenylene Ethynylene) Macrocycles: Persistent Columnar Stacking Driven by Multiple Hydrogen-Bonding Interactions. *Journal of the American Chemical Society*, **2017**, 139, 15950-15957	16.4	25

279	B-Doped MnN4-G Nanosheets as Bifunctional Electrocatalysts for Both Oxygen Reduction and Oxygen Evolution Reactions. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 18711-18717	8.3	25
278	Reexamination of the depolarized-light-scattering spectra of glass-forming liquids. *Physical Review E*, **1994**, 50, 1711-1716	2.4	25
277	In- and Ga-based inorganic double perovskites with direct bandgaps for photovoltaic applications. *Physical Chemistry Chemical Physics*, **2017**, 19, 21691-21695	3.6	24
276	Tri-Wing Graphene Nano-Paddle-Wheel with a Single-File Metal Joint: Formation of Multi-Planar Tetracoordinated-Carbon (ptC) Strips. *Journal of Physical Chemistry C*, **2012**, 116, 11378-11385	3.8	24
275	Carbon Nanotube Superarchitectures: An Ab Initio Study. *Journal of Physical Chemistry C*, **2011**, 115, 18174-18185	3.8	24
274	Ab initio prediction of amorphous B84. *Journal of Physical Chemistry A*, **2010**, 114, 2245-9	2.8	24
273	Cooperative effects in two-dimensional ring-like networks of three-center hydrogen bonding interactions. *Journal of Chemical Physics*, **2005**, 122, 184325	3.9	24
272	Time-Resolved Measurements of Photocarrier Dynamics in TiS3 Nanoribbons. *ACS Applied Materials & Interfaces*, **2016**, 8, 18334-8	9.5	24
271	An ab initio study of the nickel-catalyzed transformation of amorphous carbon into graphene in rapid thermal processing. *Nanoscale*, **2016**, 8, 9746-55	7.7	24
270	Point defects in lines in single crystalline phosphorene: directional migration and tunable band gaps. *Nanoscale*, **2016**, 8, 17801-17808	7.7	24
269	Understanding the quenching nature of Mn in wide band gap inorganic compounds: design principles for Mn phosphors with higher efficiency. *Physical Chemistry Chemical Physics*, **2018**, 20, 16992-16999	3.6	24
268	Two-Dimensional Gold Sulfide Monolayers with Direct Band Gap and Ultrahigh Electron Mobility. *Journal of Physical Chemistry Letters*, **2019**, 10, 3773-3778	6.4	23
267	Phonon thermal transport in a graphene/MoSe van der Waals heterobilayer. *Physical Chemistry Chemical Physics*, **2018**, 20, 2637-2645	3.6	23
266	Unraveling a New Chemical Mechanism of Missing Sulfate Formation in Aerosol Haze: Gaseous NO with Aqueous HSO/SO. *Journal of the American Chemical Society*, **2019**, 141, 19312-19320	16.4	23
265	Interfaces Select Specific Stereochemical Conformations: The Isomerization of Glyoxal at the Liquid Water Interface. *Journal of the American Chemical Society*, **2017**, 139, 27-30	16.4	23
264	Liquid-solid and solid-solid phase transition of monolayer water: high-density rhombic monolayer ice. *Journal of Chemical Physics*, **2014**, 140, 184507	3.9	23
263	Dipole-induced, thermally stable lamellar structure by polar aromatic silane. *Journal of the American Chemical Society*, **2009**, 131, 900-1	16.4	23
262	Gas□quid nucleation in two-dimensional fluids. *Journal of Chemical Physics*, **1996**, 104, 2699-2704	3.9	23

261	Phase transitions and ferroelasticity–multiferroicity in bulk and two-dimensional silver and copper monohalides. *Nanoscale Horizons*, **2019**, 4, 1106-1112	10.8	22
260	Mechanistic Insight into the Reaction of Organic Acids with SO at the Air-Water Interface. *Angewandte Chemie - International Edition*, **2019**, 58, 8351-8355	16.4	22
259	Unusual Magnetic Properties of Functionalized Graphene Nanoribbons. *Journal of Physical Chemistry Letters*, **2013**, 4, 2482-2488	6.4	22
258	Free-Standing All-Nanoparticle Thin Fibers: A Novel Nanostructure Bridging Zero- and One-Dimensional Nanoscale Features. *Advanced Materials*, **2009**, 21, 314-319	24	22
257	Molecular simulations of solid-liquid interfacial tension of silicon. *Journal of Chemical Physics*, **2006**, 124, 236103	3.9	22
256	Effect of apical defects and doped atoms on field emission of boron nitride nanocones. *Journal of Physical Chemistry B*, **2006**, 110, 16346-52	3.4	22
255	Probing the structures of gold-aluminum alloy clusters AuxAly(-): a joint experimental and theoretical study. *Nanoscale*, **2016**, 8, 9805-14	7.7	22
254	High ZT 2D Thermoelectrics by Design: Strong Interlayer Vibration and Complete Band-Extrema Alignment. *Advanced Functional Materials*, **2020**, 30, 2001200	15.6	21
253	Water Confined in Nanocapillaries: Two-Dimensional Bilayer Squarelike Ice and Associated Solid–Liquid–Solid Transition. *Journal of Physical Chemistry C*, **2018**, 122, 6704-6712	3.8	21
252	Al2C Monolayer Sheet and Nanoribbons with Unique Direction-Dependent Acoustic-Phonon-Limited Carrier Mobility and Carrier Polarity. *Journal of Physical Chemistry Letters*, **2016**, 7, 302-7	6.4	21
251	Integration of a functionalized graphene nano-network into a planar perovskite absorber for high-efficiency large-area solar cells. *Materials Horizons*, **2018**, 5, 868-873	14.4	21
250	Au6S2 monolayer sheets: metallic and semiconducting polymorphs. *Materials Horizons*, **2017**, 4, 1085-1091	14.4	21
249	Fluorinating Hexagonal Boron Nitride/Graphene Multilayers into Hybrid Diamondlike Nanofilms with Tunable Energy Gap. *Journal of Physical Chemistry C*, **2011**, 115, 21678-21684	3.8	21
248	Computer simulation of bilayer ice: structures and thermodynamics. *Physica A: Statistical Mechanics and Its Applications*, **2003**, 319, 163-174	3.3	21
247	Effect of an electric field on the surface tension of a dipolar-quadrupolar fluid and its implication for sign preference in droplet nucleation. *Physical Review Letters*, **2002**, 89, 246104	7.4	21
246	Statistical Mechanics of Surface Tension and Tolman Length of Dipolar Fluids. *Journal of Physical Chemistry B*, **2001**, 105, 11586-11594	3.4	21
245	Structural and magnetic evolution of bimetallic MnAu clusters driven by asymmetric atomic migration. *Nano Letters*, **2014**, 14, 1362-8	11.5	20
244	New Computational Approach to Determine Liquid-Solid Phase Equilibria of Water Confined to Slit Nanopores. *Journal of Chemical Theory and Computation*, **2013**, 9, 3299-310	6.4	20

243	Nanochannel with uniform and Janus surfaces: shear thinning and thickening in surfactant solution. *Langmuir*, **2012**, 28, 2866-72	4	20
242	Solid-Liquid Interfacial Free Energy of Water: A Molecular Dynamics Simulation Study. *Journal of Chemical Theory and Computation*, **2007**, 3, 1494-8	6.4	20
241	Formation of Quasi Two-dimensional Bilayer Ice in Hydrophobic Slits: A Possible Candidate for Ice XIII?. *Molecular Simulation*, **2003**, 29, 619-626	2	20
240	Rotational Barrier for 1,1-Difluoroethane, 1,1,1,2-Tetrafluoroethane, Pentafluoroethane, and Hexafluoroethane: A Density Functional and ab Initio Molecular Orbital Study. *Journal of Physical Chemistry A*, **1998**, 102, 654-658	2.8	20
239	A type-I van der Waals heterobilayer of WSe/MoTe. *Nanotechnology*, **2018**, 29, 335203	3.4	20
238	A molecular perspective for global modeling of upper atmospheric NH from freezing clouds. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 6147-6152	11.5	20
237	Niobium oxide dihalides NbOX2: a new family of two-dimensional van der Waals layered materials with intrinsic ferroelectricity and antiferroelectricity. *Nanoscale Horizons*, **2019**, 4, 1113-1123	10.8	19
236	Two-dimensional interlocked pentagonal bilayer ice: how do water molecules form a hydrogen bonding network?. *Physical Chemistry Chemical Physics*, **2016**, 18, 14216-21	3.6	19
235	Polygermanes: bandgap engineering via tensile strain and side-chain substitution. *Chemical Communications*, **2014**, 50, 9126-9	5.8	19
234	Amide Functionalization of Graphene and Carbon Nanotubes: Coverage- and Pattern-Dependent Electronic and Magnetic Properties. *Journal of Physical Chemistry C*, **2012**, 116, 13722-13730	3.8	19
233	[CTi7(2+)]: Heptacoordinate Carbon Motif?. *Journal of Physical Chemistry Letters*, **2012**, 3, 2264-8	6.4	19
232	Two-dimensional to three-dimensional structural transition of gold cluster Au10 during soft landing on TiO2 surface and its effect on CO oxidation. *Journal of Chemical Physics*, **2010**, 133, 134707	3.9	19
231	Size-Dependent Phase Changes in Water Clusters. *Journal of Chemical Theory and Computation*, **2011**, 7, 3083-7	6.4	19
230	Integral equation and Monte Carlo simulation studies of clusters in infinitely dilute supercritical solutions. *Chemical Physics Letters*, **1995**, 239, 168-172	2.5	19
229	Formation of Trilayer Ices in Graphene Nanocapillaries under High Lateral Pressure. *Journal of Physical Chemistry C*, **2016**, 120, 8109-8115	3.8	19
228	Au13(8e): A secondary block for describing a special group of liganded gold clusters containing icosahedral Au13 motifs. *Chemical Physics Letters*, **2017**, 675, 35-39	2.5	18
227	Molecular Insight into Different Denaturing Efficiency of Urea, Guanidinium, and Methanol: A Comparative Simulation Study. *Journal of Chemical Theory and Computation*, **2013**, 9, 2540-51	6.4	18
226	Search for lowest-energy nonclassical fullerenes III: C22. *Journal of Physical Chemistry A*, **2009**, 113, 8839-44	2.8	18

225	Crystalline ice grown on the surface of the ferroelectric polymer poly(vinylidene fluoride) (70%) and trifluoroethylene (30%). *Journal of the American Chemical Society*, **2005**, 127, 17261-5	16.4	18
224	An extension of the quasicontinuum treatment of multiscale solid systems to nonzero temperature. *Journal of Chemical Physics*, **2004**, 121, 9279-82	3.9	18
223	Coarse-graining description of solid systems at nonzero temperature. *Journal of Chemical Physics*, **2003**, 119, 8013-8023	3.9	18
222	Monte Carlo simulation of homogeneous binary vapor□liquid nucleation: Mutual enhancement of nucleation in a partially miscible system. *Journal of Chemical Physics*, **2001**, 115, 8518-8524	3.9	18
221	Molecular dynamics study of a phase-separating fluid mixture under shear flow. *Physical Review E*, **1999**, 59, 3223-3230	2.4	18
220	Catalytic Directional Cutting of Hexagonal Boron Nitride: The Roles of Interface and Etching Agents. *Nano Letters*, **2017**, 17, 3208-3214	11.5	17
219	Structural Evolution of Gold Clusters Au (n = 21-25) Revisited. *Journal of Physical Chemistry A*, **2017**, 121, 2466-2474	2.8	17
218	Lead-free low-dimensional tin halide perovskites with functional organic spacers: breaking the charge-transport bottleneck. *Journal of Materials Chemistry A*, **2019**, 7, 16742-16747	13	17
217	Tuning the Stereoselectivity and Solvation Selectivity at Interfacial and Bulk Environments by Changing Solvent Polarity: Isomerization of Glyoxal in Different Solvent Environments. *Journal of the American Chemical Society*, **2018**, 140, 5535-5543	16.4	17
216	Direct observation of 2-dimensional ices on different surfaces near room temperature without confinement. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 16723-16728	11.5	17
215	Transition-metal-molecular sandwich nanowires as magnetic on/off switch. *Applied Physics Letters*, **2011**, 99, 053121	3.4	17
214	Toward a molecular theory of vapor-phase nucleation. V. Self-consistency in the decoupled dimer limit. *Journal of Chemical Physics*, **1997**, 107, 1242-1246	3.9	17
213	Molecular dynamics simulation of supersaturated vapor nucleation in slit pore. II. Thermostatted atomic-wall model. *Journal of Chemical Physics*, **2001**, 114, 9578-9584	3.9	17
212	Effects of external electric field on the interfacial properties of weakly dipolar fluid. *Journal of Chemical Physics*, **2001**, 114, 504	3.9	17
211	Effect of carrier-gas pressure on barrier to nucleation: Monte Carlo simulation of water/nitrogen system. *Journal of Chemical Physics*, **2001**, 114, 2681-2686	3.9	17
210	Can thin disk-like ice clusters be more stable than compact droplet-like ice clusters?. *Chemical Physics Letters*, **1999**, 304, 378-384	2.5	17
209	Probing the Structural Evolution of Gold□Aluminum Bimetallic Clusters (Au2Aln□, n = 3□11) Using Photoelectron Spectroscopy and Theoretical Calculations. *Journal of Physical Chemistry C*, **2017**, 121, 18234-18243	3.8	17
208	Unexpected quenching effect on new particle formation from the atmospheric reaction of methanol with SO. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 24966-24971	11.5	17

207	Insights into High Conductivity of the Two-Dimensional Iodine-Oxidized sp-c-COF. *ACS Applied Materials & Interfaces*, **2018**, 10, 43595-43602	9.5	17
206	Reconciling the Debate on the Existence of Pentazole HN in the Pentazolate Salt of (N)(HO)(NH)Cl. *Journal of the American Chemical Society*, **2019**, 141, 2984-2989	16.4	16
205	AB-stacked square-like bilayer ice in graphene nanocapillaries. *Physical Chemistry Chemical Physics*, **2016**, 18, 22039-46	3.6	16
204	Medium-sized Au40(SR)24 and Au52(SR)32 nanoclusters with distinct gold-kernel structures and spectroscopic features. *Nanoscale*, **2016**, 8, 1299-304	7.7	16
203	Dense monolayer films of atomically precise graphene nanoribbons on metallic substrates enabled by direct contact transfer of molecular precursors. *Nanoscale*, **2017**, 9, 18835-18844	7.7	16
202	Understanding molecular motor walking along a microtubule: a themosensitive asymmetric Brownian motor driven by bubble formation. *Journal of the American Chemical Society*, **2013**, 135, 8616-24	16.4	16
201	Self-assembled nanolayers of conjugated silane with pi-pi interlocking. *ACS Nano*, **2010**, 4, 3773-80	16.7	16
200	Molecular dynamics simulations of urea-water binary droplets on flat and pillared hydrophobic surfaces. *Faraday Discussions*, **2010**, 146, 185-93; discussion 195-215, 395-403	3.6	16
199	Theoretical and experimental characterization of structures of MnAu nanoclusters in the size range of 1-3 nm. *ACS Nano*, **2011**, 5, 9966-76	16.7	16
198	The melting temperature of bulk silicon from ab initio molecular dynamics simulations. *Chemical Physics Letters*, **2009**, 481, 88-90	2.5	16
197	Search for lowest-energy structure of Zintl dianion Si(12)(2-), Ge(12)(2-), and Sn(12)(2-). *Journal of Chemical Physics*, **2008**, 128, 154326	3.9	16
196	M4 @Si28 (M=Al,Ga): metal-encapsulated tetrahedral silicon fullerene. *Journal of Chemical Physics*, **2005**, 123, 204325	3.9	16
195	Influence of atmospheric conditions on sulfuric acid-dimethylamine-ammonia-based new particle formation. *Chemosphere*, **2020**, 245, 125554	8.4	16
194	Unraveling nucleation pathway in methane clathrate formation. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 24701-24708	11.5	16
193	PbTiO3 as Electron-Selective Layer for High-Efficiency Perovskite Solar Cells: Enhanced Electron Extraction via Tunable Ferroelectric Polarization. *Advanced Functional Materials*, **2019**, 29, 1806427	15.6	16
192	PtSe Monolayer: A Highly Efficient Electrocatalyst toward Hydrogen and Oxygen Electrode Reactions. *ACS Applied Materials & Interfaces*, **2020**, 12, 13896-13903	9.5	15
191	Formation of aqueous-phase sulfate during the haze period in China: Kinetics and atmospheric implications. *Atmospheric Environment*, **2018**, 177, 93-99	5.3	15
190	Formation of CO2 Hydrates within Single-Walled Carbon Nanotubes at Ambient Pressure: CO2 Capture and Selective Separation of a CO2/H2 Mixture in Water. *Journal of Physical Chemistry C*, **2018**, 122, 7951-7958	3.8	15

189	Thin-Film Transformation of NH4PbI3 to CH3NH3PbI3 Perovskite: A Methylamine-Induced Conversion□Healing Process. *Angewandte Chemie*, **2016**, 128, 14943-14947	3.6	15
188	Structural evolution and magnetic properties of anionic clusters CrGe (n = 3-14): photoelectron spectroscopy and density functional theory computation. *Journal of Physics Condensed Matter*, **2018**, 30, 335501	1.8	15
187	Ab initio study of structural, electronic, and magnetic properties of V(n)(C(60))(m) complexes. *Journal of Physical Chemistry A*, **2009**, 113, 5406-13	2.8	15
186	Water transport through subnanopores in the ultimate size limit: Mechanism from molecular dynamics. *Nano Research*, **2019**, 12, 587-592	10	15
185	Mechanistic insights into tunable luminescence and persistent luminescence of the full-color-emitting BCNO phosphors. *Carbon*, **2017**, 122, 176-184	10.4	14
184	Au(□5)(0e) elementary block: new insights into ligated gold clusters with □sulfido motifs. *Nanoscale*, **2017**, 9, 8990-8996	7.7	14
183	Facile and Versatile Functionalization of Two-Dimensional Carbon Nitrides by Design: Magnetism/Multiferroicity, Valleytronics, and Photovoltaics. *Advanced Functional Materials*, **2019**, 29, 1905752	15.6	14
182	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie - International Edition*, **2020**, 59, 11550-11555	16.4	14
181	CO Separation from H via Hydrate Formation in Single-Walled Carbon Nanotubes. *Journal of Physical Chemistry Letters*, **2016**, 7, 4911-4915	6.4	14
180	Persistent Luminescence Hole-Type Materials by Design: Transition-Metal-Doped Carbon Allotrope and Carbides. *ACS Applied Materials & Interfaces*, **2016**, 8, 5439-44	9.5	14
179	Carbon nanotube and boron nitride nanotube hosted C60□ nanopeapods. *Journal of Materials Chemistry C*, **2013**, 1, 4518	7.1	14
178	Resonant photoemission observations and DFT study of s-d hybridization in catalytically active gold clusters on ceria nanorods. *Angewandte Chemie - International Edition*, **2013**, 52, 6936-9	16.4	14
177	Scanning Motions of an Atomic Force Microscope Tip in Water. *Physical Review Letters*, **1997**, 79, 853-856	7.4	14
176	Structure and thermophysical properties of single-wall Si nanotubes. *Physica B: Condensed Matter*, **2008**, 403, 2021-2028	2.8	14
175	Rutile TiO(011)-2□1 Reconstructed Surfaces with Optical Absorption over the Visible Light Spectrum. *ACS Applied Materials & Interfaces*, **2016**, 8, 27403-27410	9.5	14
174	Room temperature electrofreezing of water yields a missing dense ice phase in the phase diagram. *Nature Communications*, **2019**, 10, 1925	17.4	13
173	Hydration, Solvation, and Isomerization of Methylglyoxal at the Air/Water Interface: New Mechanistic Pathways. *Journal of the American Chemical Society*, **2020**, 142, 5574-5582	16.4	13
172	Structural Evolution of Gold-Doped Bismuth Clusters AuBi□(n = 4□8). *Journal of Physical Chemistry C*, **2018**, 122, 6947-6954	3.8	13

171	Formation of bilayer clathrate hydrates. *Journal of Materials Chemistry A*, **2015**, 3, 5547-5555	13	13
170	COMPUTER SIMULATION OF LIQUID□VAPOR INTERFACIAL TENSION: LENNARD-JONES FLUID AND WATER REVISITED. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 733-763	1.8	13
169	Molecularly intercalated nanoflakes: a supramolecular composite for strong energy absorption. *Advanced Materials*, **2010**, 22, 4457-61	24	13
168	Analysis of the gas states at a liquid/solid interface based on interactions at the microscopic level. *Journal of Physical Chemistry B*, **2007**, 111, 9325-9	3.4	13
167	Effects of line defects on the electronic properties of ZnO nanoribbons and sheets. *Journal of Materials Chemistry C*, **2017**, 5, 3121-3129	7.1	12
166	Au: The Smallest Gold Cluster with the High-Symmetry Icosahedral Core Au. *Journal of Physical Chemistry Letters*, **2019**, 10, 1820-1827	6.4	12
165	Covalent nitrophenyl diazonium functionalized silicene for spintronics: a first-principles study. *Physical Chemistry Chemical Physics*, **2015**, 17, 17957-61	3.6	12
164	Thermal transport in phosphorene and phosphorene-based materials: A review on numerical studies. *Chinese Physics B*, **2018**, 27, 036501	1.2	12
163	Theoretical studies on tunable electronic structures and potential applications of two-dimensional arsenene-based materials. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1387	7.9	12
162	Excitations of Precursor Molecules by Different Laser Powers in Laser-Assisted Growth of Diamond Films. *Crystal Growth and Design*, **2010**, 10, 4928-4933	3.5	12
161	Monte Carlo simulation of the solid to superliquid phase transition of Langmuir monolayers. II. Characteristics of phase transition. *Journal of Chemical Physics*, **1997**, 106, 1961-1966	3.9	12
160	Basis set effects on the intermolecular interaction of the CF4□CF4 system. *Computational and Theoretical Chemistry*, **2000**, 503, 213-220		12
159	Use of Ion Exchange To Regulate the Heterogeneous Ice Nucleation Efficiency of Mica. *Journal of the American Chemical Society*, **2020**, 142, 17956-17965	16.4	12
158	PCl: A Unique Post-Phosphorene 2D Material with Superior Properties against Oxidation. *Journal of Physical Chemistry Letters*, **2018**, 9, 6568-6575	6.4	12
157	Control of crystallographic orientation in diamond synthesis through laser resonant vibrational excitation of precursor molecules. *Scientific Reports*, **2014**, 4, 4581	4.9	11
156	Influence of Structural Fluctuations, Proton Transfer, and Electric Field on Polarization Switching of Supported Two-Dimensional Hydrogen-Bonded Oxocarbon Monolayers. *Chemistry of Materials*, **2015**, 27, 4839-4847	9.6	11
155	Co-mixing hydrogen and methane may double the energy storage capacity. *Journal of Materials Chemistry A*, **2018**, 6, 8916-8922	13	11
154	Carbon fragments as highly active metal-free catalysts for the oxygen reduction reaction: a mechanistic study. *Nanoscale*, **2019**, 11, 19422-19428	7.7	11

153	Interaction between O2 and neutral/charged Au (n= 1–8) clusters: A comparative study between density-functional theory and coupled cluster calculations. *Chemical Physics Letters*, **2014**, 592, 127-131	2.5	11
152	Phase diagrams of confined solutions of dimyristoylphosphatidylcholine (DMPC) lipid and cholesterol in nanotubes. *Microfluidics and Nanofluidics*, **2013**, 14, 995-1010	2.8	11
151	Cooperativity effects in cyclic trifluoromethanol trimer: an ab initio study. *Computational and Theoretical Chemistry*, **1998**, 431, 119-126		11
150	Gas hydrates in confined space of nanoporous materials: new frontier in gas storage technology. *Nanoscale*, **2021**, 13, 7447-7470	7.7	11
149	An ultralow-density porous ice with the largest internal cavity identified in the water phase diagram. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 12684-12691	11.5	10
148	Rational design of one-dimensional hybrid organic–inorganic perovskites with room-temperature ferroelectricity and strong piezoelectricity. *Materials Horizons*, **2019**, 6, 1463-1473	14.4	10
147	Phase behaviors of deeply supercooled bilayer water unseen in bulk water. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 4839-4844	11.5	10
146	Edge decorated SiC nanoribbons with metal: Coexistence of planar tetracoordinate carbon and silicon. *Chemical Physics Letters*, **2013**, 580, 78-81	2.5	10
145	Freezing point and solid-liquid interfacial free energy of Stockmayer dipolar fluids: a molecular dynamics simulation study. *Journal of Chemical Physics*, **2013**, 139, 114705	3.9	10
144	New phases of 3d-transition metal–cerium binary compounds: an extensive structural search. *RSC Advances*, **2017**, 7, 40486-40498	3.7	10
143	Reply to "Comment on 'two-dimensional boron monolayer sheets'". *ACS Nano*, **2013**, 7, 880-1	16.7	10
142	Reexamine structures and relative stability of medium-sized silicon clusters: Low-lying endohedral fullerene-like clusters Si30–Si38. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2009**, 373, 3757-3760	2.3	10
141	Vapour - liquid equilibria of binary mixtures containing Stockmayer molecules. *Journal of Physics Condensed Matter*, **1997**, 9, 3349-3360	1.8	10
140	Vapor-liquid equilibria for pure substances by Gibbs ensemble simulation of Stockmayer potential molecules. *Fluid Phase Equilibria*, **1997**, 137, 87-98	2.5	10
139	Quantum confinement of crystalline silicon nanotubes with nonuniform wall thickness: Implication to modulation doping. *Applied Physics Letters*, **2007**, 91, 103107	3.4	10
138	Direct synthesis of bifunctional nanorods from a Co–adenine–MoO3 hybrid for overall water splitting. *Materials Chemistry Frontiers*, **2020**, 4, 546-554	7.8	10
137	Computational Prediction of Novel Ice Phases: A Perspective. *Journal of Physical Chemistry Letters*, **2020**, 11, 7449-7461	6.4	10
136	Two-dimensional MgXSe (X = Al, Ga) monolayers with tunable electronic properties for optoelectronic and photocatalytic applications. *Nanoscale*, **2019**, 11, 19806-19813	7.7	10

135	Interaction between Iron and Graphene Nanocavity: Formation of Iron Membranes, Iron Clusters, or Iron Carbides. *ACS Applied Materials & Interfaces*, **2017**, 9, 12100-12108	9.5	9
134	Electronic and transport properties of porous graphene sheets and nanoribbons: benzo-CMPs and BN codoped derivatives. *Journal of Materials Chemistry C*, **2015**, 3, 9637-9649	7.1	9
133	Anatase (101) Reconstructed Surface with Novel Functionalities: Desired Bandgap for Visible Light Absorption and High Chemical Reactivity. *Advanced Functional Materials*, **2018**, 28, 1705529	15.6	9
132	Photovoltaic Diode Effect Induced by Positive Bias Poling of Organic Layer-Mediated Interface in Perovskite Heterostructure HC(NH2)2PbI3/TiO2. *Advanced Materials Interfaces*, **2016**, 3, 1600267	4.6	9
131	Monolayered semiconducting GeAsSe and SnSbTe with ultrahigh hole mobility. *Frontiers of Physics*, **2018**, 13, 1	3.7	9
130	Diisopropylammonium Bromide Based Two-Dimensional Ferroelectric Monolayer Molecular Crystal with Large In-Plane Spontaneous Polarization. *Journal of the American Chemical Society*, **2019**, 141, 1452-1456	16.4	9
129	Two-dimensional crystallization of hexagonal bilayer with Moir patterns. *Journal of Physical Chemistry B*, **2012**, 116, 4363-9	3.4	9
128	Homogeneous nanocables from double-walled boron-nitride nanotubes using first-principles calculations. *Physical Review B*, **2010**, 82,	3.3	9
127	Density-Functional Theory Studies of Step-Kinked Carbon Nanotubes. *Journal of Physical Chemistry C*, **2011**, 115, 4235-4239	3.8	9
126	Liquid solid phase transitions of Lennard-Jones particles confined to slit pores: towards the construction of temperature pressure-slit width phase diagram. *Molecular Simulation*, **2012**, 38, 373-377	2	9
125	Motif Transition in Growth Patterns of Small to Medium-Sized Silicon Clusters. *Angewandte Chemie*, **2005**, 117, 1515-1518	3.6	9
124	The Boundary Condition in the Gibbs Ensemble Simulation of a Stockmayer Fluid under an Applied Field. *Molecular Simulation*, **1999**, 23, 95-107	2	9
123	Effects of solute size on the local solvent density and solute solubility in infinitely dilute supercritical solutions. *Fluid Phase Equilibria*, **1996**, 116, 296-303	2.5	9
122	Modulation of the Double-Helical Cores: A New Strategy for Structural Predictions of Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry Letters*, **2020**, 11, 536-540	6.4	9
121	Electronic and transport properties of carbon and boron-nitride ferrocene nanopeapods. *Journal of Materials Chemistry C*, **2014**, 2, 10017-10030	7.1	8
120	Supramolecular Nanolayer Reconfiguration after Molecular Intercalation. *Journal of Physical Chemistry C*, **2011**, 115, 10351-10356	3.8	8
119	Effects of Radical Site Location and Surface Doping on the Radical Chain-reaction on HSi(100)-(2 1): A Density Functional Theory Study. *Journal of Physical Chemistry C*, **2008**, 112, 16078-16086	3.8	8
118	Bulk and interfacial properties of quadrupolar fluids. *Journal of Chemical Physics*, **2002**, 117, 3982-3991	3.9	8

117	Understanding the origin of phase segregation of nano-crystalline in a Be(x)Zn(1-x)O random alloy: a novel phase of Be(1/3)Zn(2/3)O. *Nanoscale*, **2015**, 7, 9852-8	7.7	7
116	Two-Dimensional AuMX (M = Al, Ga, In; X = S, Se) Monolayers Featuring Intracrystalline Aurophilic Interactions with Novel Electronic and Optical Properties. *ACS Applied Materials & Interfaces*, **2018**, 10, 16739-16746	9.5	7
115	Mechanistic study of pressure and temperature dependent structural changes in reactive formation of silicon carbonate. *RSC Advances*, **2016**, 6, 26650-26657	3.7	7
114	Electronic structure engineering in chemically modified ultrathin ZnO nanofilms via a built-in heterointerface. *RSC Advances*, **2014**, 4, 18718-18723	3.7	7
113	The electronic and transport properties of (VBz)n@CNT and (VBz)n@BNNT nanocables. *Journal of Materials Chemistry C*, **2015**, 3, 4039-4049	7.1	7
112	Silicon-Containing Multidecker Organometallic Complexes and Nanowires: A Density Functional Theory Study. *Journal of Physical Chemistry Letters*, **2012**, 3, 151-156	6.4	7
111	Metal-organic frameworks capable of healing at low temperatures. *Advanced Materials*, **2013**, 25, 6106-11	24	7
110	Solvent-induced interactions between hydrophobic and hydrophilic polyatomic sheets in water and hypothetical nonpolar water. *Journal of Chemical Physics*, **1997**, 106, 9781-9792	3.9	7
109	Hybrid atomistic-coarse-grained treatment of thin-film lubrication. I. *Journal of Chemical Physics*, **2004**, 120, 6744-50	3.9	7
108	Computer simulation of water ice transition in hydrophobic nanopores. *Physica A: Statistical Mechanics and Its Applications*, **2001**, 292, 87-101	3.3	7
107	Monte Carlo simulation of vapor liquid binodal of water. *Journal of Chemical Physics*, **2002**, 117, 9518-9519	3.9	7
106	Can the van der Waals loop vanish?. *Chemical Physics Letters*, **1994**, 231, 401-406	2.5	7
105	Atomically Resolved Electrically Active Intragrain Interfaces in Perovskite Semiconductors.. *Journal of the American Chemical Society*, **2022**,	16.4	7
104	Turning a Superhydrophilic Surface Weakly Hydrophilic: Topological Wetting States. *Journal of the American Chemical Society*, **2020**, 142, 18491-18502	16.4	7
103	Large magnetic anisotropy in chemically engineered iridium dimer. *Communications Physics*, **2018**, 1,	5.4	7
102	Two-Dimensional IV-V Monolayers with Highly Anisotropic Carrier Mobility and Electric Transport Properties. *Journal of Physical Chemistry Letters*, **2021**, 12, 1058-1065	6.4	7
101	New Insights into the Stability of Anhydrous 2-Imidazolium Fluoride and its High Dissolution Capability toward a Strongly Hydrogen-Bonded Compound. *Journal of the American Chemical Society*, **2020**, 142, 10314-10318	16.4	6
100	PtCoNi Alloy Nanoclusters for Synergistic Catalytic Oxygen Reduction Reaction. *ACS Applied Nano Materials*, **2020**, 3, 2536-2544	5.6	6

99	Fundamental measure density functional theory study of liquid-vapor interface of dipolar and quadrupolar fluids. *Journal of Chemical Physics*, **2013**, 139, 134502	3.9	6
98	Unraveling Crystalline Structure of High-Pressure Phase of Silicon Carbonate. *Physical Review X*, **2014**, 4,	9.1	6
97	Static Frictional Forces at Crystalline Interfaces. *Journal of Physical Chemistry B*, **1997**, 101, 4992-4997	3.4	6
96	The effect of a uniform electric field on homogeneous vapor–liquid nucleation in a dipolar fluid. I. Stockmayer fluid. *Journal of Chemical Physics*, **1998**, 109, 8435-8441	3.9	6
95	Contribution of the center-of-mass fluctuation of a liquid cluster to the free energy: A Monte Carlo simulation study. *Journal of Chemical Physics*, **1998**, 108, 4683-4684	3.9	6
94	The effective-medium approximation for the thermoelectric power of polycrystals: application to a model for La2-xMxCuO4. *Journal of Physics C: Solid State Physics*, **1987**, 20, L907-L910		6
93	Towards complete assignment of the infrared spectrum of the protonated water cluster H(HO). *Nature Communications*, **2021**, 12, 6141	17.4	6
92	Chiral Au(SR): a new ligand-binding strategy for structural prediction of thiolate-protected gold nanocluster. *Chemical Communications*, **2020**, 56, 2995-2998	5.8	6
91	Molecular Design of Three-Dimensional Metal-Free A(NH)X Perovskites for Photovoltaic Applications. *Jacs Au*, **2021**, 1, 475-483		6
90	Structural, electronic and mechanical properties of sp-hybridized BN phases. *Physical Chemistry Chemical Physics*, **2017**, 19, 9923-9933	3.6	5
89	Tuning electronic structure of monolayer InP in contact with graphene or Ni: effect of a buffer layer and intrinsic In and P-vacancy. *Physical Chemistry Chemical Physics*, **2019**, 21, 1285-1293	3.6	5
88	Bi(Sb)NCa3: Expansion of Perovskite Photovoltaics into All-Inorganic Anti-Perovskite Materials. *Journal of Physical Chemistry C*, **2019**, 123, 6363-6369	3.8	5
87	Molecular dynamics simulation of heterogeneous nucleation on nanotubes. *RSC Advances*, **2015**, 5, 40953-40963	3.7	5
86	The freezing tendency towards 4-coordinated amorphous networks causes an increase in the heat capacity of supercooled Stillinger–Weber silicon. *RSC Advances*, **2015**, 5, 44679-44686	3.7	5
85	Abnormal phase transition between two-dimensional high-density liquid crystal and low-density crystalline solid phases. *Nature Communications*, **2018**, 9, 198	17.4	5
84	Monopolar Magnetic MOF-74 with Hybrid Node NiFe. *Journal of Physical Chemistry C*, **2016**, 120, 26908-26914	3.8	5
83	Correspondence: Reply to 'On the bonding in ligand-protected gold clusters'. *Nature Communications*, **2017**, 8, 1351	17.4	5
82	Tunable magnetism on Si(111)(21) via chemisorption of graphene nanoribbons. *Physical Review B* , **2010**, 82,	3.3	5

81	Covalent reinforcement of hydrogen-bonded discs into stably folded helical structures. *Organic Letters*, **2011**, 13, 4008-11	6.2	5
80	Coarse-grained free-energy-functional treatment of quasistatic multiscale processes in heterogeneous materials. *Journal of Chemical Physics*, **2005**, 123, 164109	3.9	5
79	Bubble Nucleation in Confined Liquids: Molecular Dynamics Study. *Progress of Theoretical Physics Supplement*, **2000**, 138, 732-733		5
78	Imaging point defects in a liquid environment: A model AFM study. *Physical Review B*, **1999**, 60, 14328-14333	3.7	5
77	Rich topologies of monolayer ices via unconventional electrowetting. *Nanoscale Horizons*, **2020**, 5, 514-522	12.8	5
76	Exploration of Formation and Size-Evolution Pathways of Thiolate-Gold Nanoclusters in the CO-Directed [Au (SR)] Synthesis. *Small*, **2021**, 17, e2000627	11	5
75	Ring Model for Understanding How Interfacial Interaction Dictates the Structures of Protection Motifs and Gold Cores in Thiolate-Protected Gold Nanoclusters. *Journal of Physical Chemistry Letters*, **2021**, 12, 3006-3013	6.4	5
74	First-Principles Molecular Dynamics Simulations of the Spontaneous Freezing Transition of 2D Water in a Nanoslit. *Journal of the American Chemical Society*, **2021**, 143, 8177-8183	16.4	5
73	Two-dimensional dry ices with rich polymorphic and polyamorphic phase behavior. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 10263-10268	11.5	5
72	Determination of CO Adsorption Sites on Gold Clusters Au (n = 21-25): A Size Region That Bridges the Pyramidal and Core-Shell Structures. *Journal of Physical Chemistry Letters*, **2018**, 9, 5430-5439	6.4	5
71	Reaction mechanism between small-sized Ce clusters and water molecules: an ab initio investigation on Ce + HO. *Physical Chemistry Chemical Physics*, **2019**, 21, 4006-4014	3.6	4
70	Structure transition of Au18 from pyramidal to a hollow-cage during soft-landing onto a TiO2(110) surface. *Chemical Communications*, **2015**, 51, 9535-8	5.8	4
69	Heterogeneous Reactions of SO on Ice: An Overlooked Sink for SO Depletion. *Journal of the American Chemical Society*, **2020**, 142, 2150-2154	16.4	4
68	Role of vacancies to p-type semiconducting properties of SiGe nanowires. *Journal of Materials Chemistry C*, **2014**, 2, 6536-6546	7.1	4
67	Controlling Cross Section of Carbon Nanotubes via Selective Hydrogenation. *Journal of Physical Chemistry C*, **2010**, 114, 11753-11757	3.8	4
66	Effects of the co-solvent energy parameter and dipolar strength on solute residual chemical potential. *Fluid Phase Equilibria*, **1997**, 138, 61-68	2.5	4
65	Multiscale treatment of thin-film lubrication. *Molecular Simulation*, **2005**, 31, 811-815	2	4
64	Hybrid atomistic-coarse-grained treatment of thin-film lubrication. II. *Journal of Chemical Physics*, **2004**, 121, 8029-38	3.9	4

63	Role of hysteresis in the molecular picture of friction. *Physical Chemistry Chemical Physics*, **2001**, 3, 1175-1178	3.6	4
62	Nonlinear effects of physisorption on static friction. *Journal of Chemical Physics*, **2000**, 113, 11293-11296	3.9	4
61	Calculation of the surface tension of liquid metals using a one-component-plasma reference system. *Journal of Physics F: Metal Physics*, **1987**, 17, 2345-2352		4
60	AgBiS2 as a low-cost and eco-friendly all-inorganic photovoltaic material: nanoscale morphology□property relationship. *Nanoscale Advances*, **2020**, 2, 770-776	5.1	4
59	Peroxo Species Formed in the Bulk of Silicate Cathodes. *Angewandte Chemie - International Edition*, **2021**, 60, 10056-10063	16.4	4
58	Unravelling the Role of Topological Defects on Catalytic Unzipping of Single-Walled Carbon Nanotubes by Single Transition Metal Atom. *Journal of Physical Chemistry Letters*, **2018**, 9, 6801-6807	6.4	4
57	Two-dimensional monolayer salt nanostructures can spontaneously aggregate rather than dissolve in dilute aqueous solutions. *Nature Communications*, **2021**, 12, 5602	17.4	4
56	Multiscale simulation on shearing transitions of thin-film lubrication with multi-layer molecules. *Chemical Physics Letters*, **2017**, 679, 6-14	2.5	3
55	Mechanistic Insight into the Reaction of Organic Acids with SO3 at the Air□Water Interface. *Angewandte Chemie*, **2019**, 131, 8439-8443	3.6	3
54	Reaction mechanism between small-sized Ce clusters and water molecules II: an ab initio investigation on Ce (n = 1-3) + mHO (m = 2-6). *Physical Chemistry Chemical Physics*, **2019**, 21, 8945-8955	3.6	3
53	Photodetectors: High-Gain and Low-Driving-Voltage Photodetectors Based on Organolead Triiodide Perovskites (Adv. Mater. 11/2015). *Advanced Materials*, **2015**, 27, 1967-1967	24	3
52	Quantitative Prediction of Aggregation-Induced Emission: A Full Quantum Mechanical Approach to the Optical Spectra. *Angewandte Chemie*, **2020**, 132, 11647-11652	3.6	3
51	A possible unaccounted source of atmospheric sulfate formation: amine-promoted hydrolysis and non-radical oxidation of sulfur dioxide. *Chemical Science*, **2020**, 11, 2093-2102	9.4	3
50	Domain Wall Conduction in Calcium-Modified Lead Titanate for Polarization Tunable Photovoltaic Devices. *Cell Reports Physical Science*, **2020**, 1, 100043	6.1	3
49	Surprising impact of remote groups on the folding--unfolding and dimer-chain equilibria of bifunctional H-bonding unimers. *Chemical Communications*, **2016**, 52, 3773-6	5.8	3
48	Homogenous Alloys of Formamidinium Lead Triiodide and Cesium Tin Triiodide for Efficient Ideal-Bandgap Perovskite Solar Cells. *Angewandte Chemie*, **2017**, 129, 12832-12836	3.6	3
47	Experimental and theoretical studies of hydroxyl-induced magnetism in TiO nanoclusters. *Nanoscale*, **2012**, 4, 7704-11	7.7	3
46	Understanding Liquid□Solid-Like Behavior of Tetrahydrofuran Adlayers at Room Temperature between Graphene and Mica: A Born□Oppenheimer Molecular Dynamics Study. *Journal of Physical Chemistry C*, **2013**, 117, 21894-21900	3.8	3

45	Molecular Dynamics Simulations of Thermal Conductivity of Silicon Nanotubes. *Journal of Computational and Theoretical Nanoscience*, **2006**, 3, 824-829	0.3	3
44	Comment on Dual-Hard-Sphere Models for Liquid Semiconductors Si And Ge. *Physics and Chemistry of Liquids*, **1989**, 19, 69-72	1.5	3
43	Constructing Stable and Potentially High-Performance Hybrid Organic-Inorganic Perovskites with "Unstable" Cations. *Research*, **2020**, 2020, 1986576	7.8	3
42	Directional Proton Transfer in the Reaction of the Simplest Criegee Intermediate with Water Involving the Formation of Transient HO. *Journal of Physical Chemistry Letters*, **2021**, 12, 3379-3386	6.4	3
41	How O-Binding Affects Structural Evolution of Medium Even-Sized Gold Clusters Au (= 20-34). *Journal of Physical Chemistry Letters*, **2021**, 12, 3560-3570	6.4	3
40	Resolving the HONO formation mechanism in the ionosphere via ab initio molecular dynamic simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 4629-33	11.5	3
39	Understanding Hygroscopic Nucleation of Sulfate Aerosols: Combination of Molecular Dynamics Simulation with Classical Nucleation Theory. *Journal of Physical Chemistry Letters*, **2019**, 10, 1126-1132	6.4	3
38	Anisotropic Properties of Quasi-1D In4Se3: Mechanical Exfoliation, Electronic Transport, and Polarization-Dependent Photoresponse. *Advanced Functional Materials*,2106459	15.6	3
37	Boron-nitride and aluminum-nitride "Pringles" and flapping motion. *Chemical Communications*, **2014** , 50, 7444-6	5.8	2
36	Molecular dynamics simulation of heterogeneous nucleation on nanorods **2013**,		2
35	Unraveling Molecular Mechanism on Dilute Surfactant Solution Controlled Ice Recrystallization. *Langmuir*, **2020**, 36, 1691-1698	4	2
34	Communication: Interaction of BrO radical with the surface of water. *Journal of Chemical Physics*, **2016**, 145, 241102	3.9	2
33	Iron Clusters Embedded in Graphene Nanocavities: Heat-Induced Structural Evolution and Catalytic C□ Bond Breaking. *ACS Applied Nano Materials*, **2019**, 2, 535-545	5.6	2
32	Criegee intermediate inside fullerene cage: Evidence for size-dependent reactivity. *Journal of Chemical Physics*, **2018**, 148, 244301	3.9	2
31	Embedded silicene nanostructures in partly-dehydrogenated polysilane. *Physical Chemistry Chemical Physics*, **2017**, 19, 10401-10405	3.6	1
30	A New Class of Bifunctional Perovskites BaMX4 (M = Co, Ni, Fe, Mn; X = F, Cl, Br, I): An n-Type Semiconductor with Combined Multiferroic and Photovoltaic Properties. *Journal of Physical Chemistry C*, **2019**, 123, 14303-14311	3.8	1
29	Method To Implement Interaction Surfaces with Virtual Companion Particles for Molecular Dynamics Simulations. *Journal of Chemical & Engineering Data*, **2019**, 64, 3693-3700	2.8	1
28	Hybrid nanobud-array structures (C24)n/MoS2 and (C24V)n/MoS2: two-dimensional half metallic and ferromagnetic materials. *Journal of Materials Chemistry C*, **2018**, 6, 3373-3386	7.1	1

27	Perovskite Solar Cells: Stable Formamidinium-Based Perovskite Solar Cells via In Situ Grain Encapsulation (Adv. Energy Mater. 22/2018). *Advanced Energy Materials*, **2018**, 8, 1870101	21.8	1
26	Magnetism in bimetallic PtxNiN clusters via cross-atomic coupling. *Journal of Materials Chemistry C*, **2019**, 7, 9293-9300	7.1	1
25	Graphene-Based Architecture and Assemblies **2013**, 153-182		1
24	Resonant Photoemission Observations and DFT Study of s Hybridization in Catalytically Active Gold Clusters on Ceria Nanorods. *Angewandte Chemie*, **2013**, 125, 7074-7077	3.6	1
23	Tunable Bandgaps: Simulation Evidence of Hexagonal-to-Tetragonal ZnSe Structure Transition: A Monolayer Material with a Wide-Range Tunable Direct Bandgap (Adv. Sci. 12/2015). *Advanced Science*, **2015**, 2,	13.6	1
22	Efficient electron and hole doping in compositionally abrupt Si/Ge nanowires. *Nanoscale*, **2013**, 5, 3880-8	7.7	1
21	Exohedral Silicon Fullerenes: Si60Pn60 and Si80Pn60 (Pn = P, As, Sb and Bi). *Journal of Cluster Science*, **2011**, 22, 343-354	3	1
20	Mechanical Properties of Nanostructured hard coating of ZrO2. *Materials Research Society Symposia Proceedings*, **2009**, 1224, 1		1
19	Study of hydrophillic interactions between polyatomic sheets in water. *Fluid Phase Equilibria*, **1998**, 144, 377-385	2.5	1
18	Density Functional Mean Field Theory of Crystal-Melt Interfaces. *Physics and Chemistry of Liquids*, **1989**, 20, 39-43	1.5	1
17	Large-Sized Au Core-Shell Clusters (= 61-66): Enduring Structure of the Icosahedral Au Core.. *Journal of Physical Chemistry Letters*, **2022**, 1389-1397	6.4	1
16	Multiturn Hollow Helices: Synthesis and Folding of Long Aromatic Oligoamides. *Organic Letters*, **2020**, 22, 6938-6942	6.2	1
15	Polysilane-Wrapped Carbon and Boron-Nitride Nanotubes: Effects of B or P Doping on Electron Transport. *Journal of Physical Chemistry C*, **2016**, 120, 5741-5754	3.8	1
14	Structural and Electronic Properties of Binary Clusters SiGe (+ = 6-13). *Journal of Nanoscience and Nanotechnology*, **2019**, 19, 7879-7885	1.3	1
13	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO on the Surface of a Water Droplet. *Angewandte Chemie - International Edition*, **2021**, 60, 20200-20203	16.4	1
12	Peroxo Species Formed in the Bulk of Silicate Cathodes. *Angewandte Chemie*, **2021**, 133, 10144-10151	3.6	0
11	Mechanistic Study of the Aqueous Reaction of Organic Peroxides with HSO3 on the Surface of a Water Droplet. *Angewandte Chemie*, **2021**, 133, 20362-20365	3.6	0
10	Formation of dimethyl carbonate direct esterification of CO with methanol on reduced or stoichiometric CeO(111) and (110) surfaces. *Physical Chemistry Chemical Physics*, **2021**, 23, 16150-16156	3.6	0

9	Anomalous Phase Behaviors of Monolayer NaCl Aqueous Solutions Induced by Effective Coulombic Interactions within Angstrom-Scale Slits.. *Journal of Physical Chemistry Letters*, **2022**, 2704-2710	6.4	0
8	Van der Waals Magnetic Heterojunctions with Giant Zero-Bias Tunneling Magnetoresistance and Photo-Assisted Magnetic Memory. *Advanced Functional Materials*,2200154	15.6	0
7	R□ktitelbild: Homogenous Alloys of Formamidinium Lead Triiodide and Cesium Tin Triiodide for Efficient Ideal-Bandgap Perovskite Solar Cells (Angew. Chem. 41/2017). *Angewandte Chemie*, **2017**, 129, 12966-12966	3.6	
6	Homogeneous connectivity of potential energy network in a solidlike state of water cluster. *Journal of Chemical Physics*, **2013**, 138, 244301	3.9	
5	Metall□rganic Frameworks: Metall□rganic Frameworks Capable of Healing at Low Temperatures (Adv. Mater. 42/2013). *Advanced Materials*, **2013**, 25, 6148-6148	24	
4	Efficient synthesis and conformational investigations of cis-pentacenediols. *Tetrahedron Letters*, **2010**, 51, 5732-5735	2	
3	Two-Dimensional GeC with Tunable Electronic and Carrier Transport Properties and a High Current ON/OFF Ratio. *Journal of Physical Chemistry Letters*, **2021**, 12, 11488-11496	6.4	
2	Innentitelbild: Peroxo Species Formed in the Bulk of Silicate Cathodes (Angew. Chem. 18/2021). *Angewandte Chemie*, **2021**, 133, 9814-9814	3.6	
1	Multiple Wetting-Dewetting States of a Water Droplet on Dual-Scale Hierarchical Structured Surfaces. *Jacs Au*, **2021**, 1, 955-966		