Minh Tho Nguyen

List of Publications by Year in Descending Order

661 papers	13,610 citations	51 h-index	73 g-index
694 ext. papers	14,574 ext. citations	3.3 avg, IF	6.72 L-index

#	Paper	IF	Citations
661	A Cluster Model for Interpretation of Surface-Enhanced Raman Scattering of Organic Compounds Interacting with Silver Nanoparticles **2022**, 255-285		
660	First-row transition metal doped germanium clusters GeM: some remarkable superhalogens.. *RSC Advances*, **2022**, 12, 13487-13499	3.7	0
659	The lowest-energy structure of the gold cluster Au: planar nonplanar?. *Physical Chemistry Chemical Physics*, **2021**, 24, 42-47	3.6	1
658	Theoretical Aspects of Nonconventional Hydrogen Bonds in the Complexes of Aldehydes and Hydrogen Chalcogenides. *Journal of Physical Chemistry A*, **2021**, 125, 10291-10302	2.8	1
657	Strontium stannate as an alternative anode for Na- and K-Ion batteries: A theoretical study. *Journal of Physics and Chemistry of Solids*, **2021**, 110505	3.9	0
656	Growth pattern of doubly metal doped silicon clusters M2Sin with M2 = Mo2, Nb2, Ta2, W2, NbMo, TaW and n = 11□18. Formation of fused cages M2Si18. *Chemical Physics Letters*, **2021**, 787, 139229	2.5	0
655	The binary aluminum scandium clusters Al Sc with + = 13: when is the icosahedron retained?. *RSC Advances*, **2021**, 11, 40072-40084	3.7	0
654	The binary boron lithium clusters BLi with = 1-14: in search for hydrogen storage materials. *Physical Chemistry Chemical Physics*, **2021**, 23, 24866-24877	3.6	1
653	Theoretical Study of the Binding of the Thiol-Containing Cysteine Amino Acid to the Silver Surface Using a Cluster Model. *Journal of Physical Chemistry A*, **2021**, 125, 3244-3256	2.8	5
652	A theoretical design of bipolar host materials for blue phosphorescent OLED. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107845	2.8	1
651	Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries. *Journal of Physical Chemistry C*, **2021**, 125, 14947-14956	3.8	1
650	Insights into adsorptive interactions between antibiotic molecules and rutile-TiO2 (110) surface. *Surface Science*, **2021**, 703, 121723	1.8	2
649	Structure, stability and bonding of the leapfrog B. *Journal of Computational Chemistry*, **2021**, 42, 72-80	3.5	1
648	Enhanced Li-ion transport in divalent metal-doped LiSnO. *Dalton Transactions*, **2021**, 50, 3020-3026	4.3	1
647	An octacoordinated Nb atom in the NbAlH cluster. *Chemical Communications*, **2021**, 57, 9518-9521	5.8	0
646	Comment on 'Structural characterization, reactivity and vibrational properties of silver clusters: a new global minimum for Ag' by P. L. Rodr□guez-Kessler, A. R. Rodr□guez-Dom□nguez, D. MacLeod Carey and A. Mu□z-Castro, Phys. Chem. Chem. Phys., 2020, 22, 27255, DOI: D0CP04018E. *Physical Chemistry Chemical Physics*, **2021**, 23, 12900-12903	3.6	2
645	Gold nanoclusters as prospective carriers and detectors of pramipexole.. *RSC Advances*, **2021**, 11, 16619-16632	3.7	5

644	Another look at the structure of the (H2O)n− system: water anion vs. hydrated electron. *Structural Chemistry*, **2021**, 32, 655-665	1.8	1
643	Another look at energetically quasi-degenerate structures of the gold cluster Au with q´=´1, 0, -1. *Journal of Computational Chemistry*, **2021**, 42, 2145-2153	3.5	3
642	Design of fused bithiophene systems containing silole and five-membered heterocycles for optoelectronic materials. *Chemical Physics Letters*, **2021**, 139093	2.5	0
641	SERS Chemical Enhancement of 2,4,5-Trichlorophenoxyacetic Acid Adsorbed on Silver Substrate. *Journal of Physical Chemistry A*, **2021**, 125, 8529-8541	2.8	2
640	Influence of Fluorination on Energetic Parameters of Silole, Phosphole, Thiophene, Oligomers of Silole and Related Acenes. *Journal of Fluorine Chemistry*, **2020**, 240, 109665	2.1	0
639	Interplay between π-Holes, Anion···H-C, and Cation-π Interactions in Dibromo[2,2]paracyclophane Complexes. *Journal of Physical Chemistry A*, **2020**, 124, 4379-4389	2.8	0
638	Molecular structure, IR, Raman and UV-VIS spectra of 2-cyanothiophene and 3-cyanothiophene: A comparative quantum chemical investigation. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 239, 118393	4.4	5
637	The teetotum cluster LiFeB and its possible use for constructing boron nanowires. *Physical Chemistry Chemical Physics*, **2020**, 22, 15013-15021	3.6	2
636	A remarkable mixture of germanium with phosphorus and arsenic atoms making stable pentagonal hetero-prisms [M@GeE], E = P, As and M = Fe, Ru, Os.. *RSC Advances*, **2020**, 10, 19781-19789	3.7	3
635	Optoelectronic properties of heptacene, its fluorinated derivatives and silole, thiophene analogues. *Materials Today Communications*, **2020**, 24, 101054	2.5	
634	Electronic Structure and Properties of Silicon-Doped Boron Clusters BnSi with n = 15−24 and Their Anions. *Journal of Physical Chemistry C*, **2020**, 124, 6770-6783	3.8	5
633	Theoretical Study of a Class of Organic D-π-A Dyes for Polymer Solar Cells: Influence of Various π-Spacers. *Crystals*, **2020**, 10, 163	2.3	4
632	Hydrogen Adsorption and Dissociation on AlnRh2+ (n = 1 to 9) Clusters: Steric and Coordination Effects. *Journal of Physical Chemistry C*, **2020**, 124, 7624-7633	3.8	4
631	Structures, stabilities and aromatic properties of endohedrally transition metal doped boron clusters M@B, M = Sc and Ti: a theoretical study. *Physical Chemistry Chemical Physics*, **2020**, 22, 8077-8087	3.6	5
630	Na- and K-Doped Li2SiO3 as an Alternative Solid Electrolyte for Solid-State Lithium Batteries. *Journal of Physical Chemistry C*, **2020**, 124, 4982-4988	3.8	5
629	Impact of the Astaxanthin, Betanin, and EGCG Compounds on Small Oligomers of Amyloid Aβ Peptide. *Journal of Chemical Information and Modeling*, **2020**, 60, 1399-1408	6.1	10
628	Silole and selenophene-based D-π-A dyes in dye-sensitized solar cells: Insights from optoelectronic and regeneration properties. *Dyes and Pigments*, **2020**, 176, 108243	4.6	3
627	A molecular level insight into adsorption of β-lactam antibiotics on vermiculite surface. *Surface Science*, **2020**, 695, 121588	1.8	4

626	Elucidating the binding mechanism of thione-containing mercaptopurine and thioguanine drugs to small gold clusters. *Journal of Computational Chemistry*, **2020**, 41, 1748-1758	3.5	5
625	Advances in Synthesis of Extended Benzosilole Derivatives and Their Analogs. *Molecules*, **2020**, 25,	4.8	10
624	Jahn-Teller and Pseudo Jahn-Teller Effects: Influences on the Electronic Structures of Small Transition, Main Group and Mixed Metal Clusters. *Structural Chemistry*, **2020**, 31, 7-23	1.8	
623	Structures and Magnetism of Cationic Chromium Manganese Bimetallic Oxide Clusters. *Journal of Physical Chemistry C*, **2020**, 124, 2598-2608	3.8	2
622	Theoretical study on the interaction of iodide electrolyte/organic dye with the TiO surface in dye-sensitized solar cells. *Physical Chemistry Chemical Physics*, **2020**, 22, 26410-26418	3.6	4
621	Theoretical investigation of protonated thiophene and two of its nitrile substituted derivatives (2-cyanothiophene and 3-cyanothiophene). *Physical Chemistry Chemical Physics*, **2020**, 22, 24735-24743	3.6	1
620	Structural Evolution and Stability Trend of Small-Sized Gold Clusters Au (= 20-30). *Journal of Physical Chemistry A*, **2020**, 124, 1289-1299	2.8	18
619	Structural, electronic, and optical properties of some new dithienosilole derivatives. *Structural Chemistry*, **2020**, 31, 2215-2225	1.8	0
618	Substituent Effects on the N-H Bond Dissociation Enthalpies, Ionization Energies, Acidities, and Radical Scavenging Behavior of 3,7-Disubstituted Phenoxazines and 3,7-Disubstituted Phenothiazines. *ACS Omega*, **2020**, 5, 27572-27581	3.9	0
617	Boosting Li-Ion Transport in Transition-Metal-Doped LiSnO. *Inorganic Chemistry*, **2020**, 59, 11841-11846	5.1	5
616	SERS Spectra of the Pesticide Chlorpyrifos Adsorbed on Silver Nanosurface: The Ag20 Cluster Model. *Journal of Physical Chemistry C*, **2020**, 124, 21702-21716	3.8	14
615	Structure and Stability of a Trefoil Leaf Motif of Metal-Doped Silicon and Germanium Clusters: M@E with E = Si and Ge and M = Fe, Ru, and Os. *Journal of Physical Chemistry A*, **2020**, 124, 8488-8495	2.8	
614	Autocatalysis in Formose Reaction and Formation of RNA Nucleosides. *Journal of Physical Chemistry B*, **2020**, 124, 11324-11336	3.4	1
613	BxGe120/+ Clusters with x = 12: Germanium Tubes Stabilized by Three and Four Boron Dopants. *Journal of Physical Chemistry C*, **2019**, 123, 24676-24684	3.8	3
612	Lithium- and sodium-ion transport properties of Li2Ti6O13, Na2Ti6O13 and Li2Sn6O13. *Journal of Solid State Chemistry*, **2019**, 279, 120930	3.3	3
611	Formation of the MB Teetotum Boron Clusters with 4d and 5d Transition Metals M = Rh, Pd, Ir, and Pt. *Journal of Physical Chemistry A*, **2019**, 123, 8170-8178	2.8	7
610	Structure, stability, absorption spectra and aromaticity of the singly and doubly silicon doped aluminum clusters Al Si with = 3-16 and = 1, 2.. *RSC Advances*, **2019**, 9, 27208-27223	3.7	4
609	Valence bonds in planar and quasi-planar boron disks. *Physical Chemistry Chemical Physics*, **2019**, 21, 729-735	3.6	2

608	Remarkable shifts of C -H and O-H stretching frequencies and stability of complexes of formic acid with formaldehydes and thioformaldehydes. *Journal of Computational Chemistry*, **2019**, 40, 1387-1400	3.5	6
607	Hydrogen Chemisorption on Doubly Vanadium Doped Aluminum Clusters. *Zeitschrift Fur Physikalische Chemie*, **2019**, 233, 799-812	3.1	6
606	A theoretical approach to the role of different types of electrons in planar elongated boron clusters. *Physical Chemistry Chemical Physics*, **2019**, 21, 13030-13039	3.6	7
605	Comment on "Theoretical Investigations on Geometrical and Electronic Structures of Silver Clusters". *Journal of Computational Chemistry*, **2019**, 40, 1990-1993	3.5	3
604	Structural Investigation of Human Prolactin Receptor Transmembrane Domain Homodimerization in a Membrane Environment through Multiscale Simulations. *Journal of Physical Chemistry B*, **2019**, 123, 4858-4866	3.4	1
603	Implications of Oxygen□Sulfur Exchange on Structural, Electronic Properties, and Stability of Alkali-Metal Hexatitanates. *Physica Status Solidi (B): Basic Research*, **2019**, 256, 1800568	1.3	2
602	Impressive capacity of the B7□and V2B7 clusters for CO2 capture. *Chemical Physics Letters*, **2019**, 728, 186-194	2.5	6
601	A model study on the mechanism and kinetics for the dissociation of water anion. *International Journal of Chemical Kinetics*, **2019**, 51, 610-617	1.4	2
600	Formation of the quasi-planar B boron cluster: topological path from B and disk aromaticity. *Physical Chemistry Chemical Physics*, **2019**, 21, 7039-7044	3.6	9
599	Effects of single and double nickel doping on boron clusters: stabilization of tubular structures in BNi, n = 2-22, m = 1, 2. *Physical Chemistry Chemical Physics*, **2019**, 21, 8365-8375	3.6	16
598	The scandium doped boron cluster BSc: a fruit can-like structure. *Physical Chemistry Chemical Physics*, **2019**, 21, 8933-8939	3.6	9
597	A model study on the mechanism and kinetics for reactions of the hydrated electron with H3O+ and NH4+ ions. *Chemical Physics Letters*, **2019**, 731, 136604	2.5	3
596	Influence of Oxygen□Sulfur Exchange on the Structural, Electronic, and Stability Properties of Alkali Hexastannates. *Journal of Physical Chemistry C*, **2019**, 123, 24375-24382	3.8	2
595	Effects of Electric Field on the Performance of Graphene-Based Counter Electrodes for Dye-Sensitized Solar Cells: A Theoretical Study. *Journal of Physical Chemistry C*, **2019**, 123, 30373-30381	3.8	4
594	Geometry and bonding of small binary boron-aluminum clusters BnAln (n = 1□7): Electron donation and interlocking aromaticity. *Chemical Physics Letters*, **2019**, 714, 87-93	2.5	3
593	Insights into the cooperativity between multiple interactions of dimethyl sulfoxide with carbon dioxide and water. *Journal of Computational Chemistry*, **2019**, 40, 464-474	3.5	9
592	B@Si: strong stabilizing effects of a triatomic cyclic boron unit on tubular silicon clusters. *Physical Chemistry Chemical Physics*, **2018**, 20, 7588-7592	3.6	12
591	Cover Image, Volume 86, Issue 4. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, C1-C1	4.2	

590	Reaction Routes for Experimentally Observed Intermediates in the Prebiotic Formation of Nucleobases under High-Temperature Conditions. *Journal of Physical Chemistry A*, **2018**, 122, 2992-3003	2.8	6
589	Lithium Hexastannate: A Potential Material for Energy Storage. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1700669	1.3	11
588	Propafenone effects on the stable structures of A16-22 system. *Chemical Physics Letters*, **2018**, 696, 55-60	2.5	4
587	Molecular details of spontaneous insertion and interaction of HCV non-structure 3 protease protein domain with PIP2-containing membrane. *Proteins: Structure, Function and Bioinformatics*, **2018**, 86, 423-433	4.2	1
586	Aromaticity of Some Metal Clusters: A Different View from Magnetic Ring Current. *Journal of Physical Chemistry A*, **2018**, 122, 1378-1391	2.8	6
585	A theoretical design of some silole-based dibenzothiophene-S,S-dioxide semiconducting compounds for red phosphorescence. *Organic Electronics*, **2018**, 54, 270-276	3.5	4
584	Insight into the adsorption of chloramphenicol on a vermiculite surface. *Chemical Physics Letters*, **2018**, 699, 107-114	2.5	8
583	Another Look at Photoelectron Spectra of the Anion CrO: Multireference Character and Energetic Degeneracy. *Journal of Chemical Theory and Computation*, **2018**, 14, 4833-4843	6.4	5
582	Size Dependent H2 Adsorption on AlnRh+ (n = 112) Clusters. *Journal of Physical Chemistry C*, **2018**, 122, 18247-18255	3.8	18
581	Elucidation of the molecular and electronic structures of some magic silver clusters Ag (n = 8, 18, 20). *Journal of Molecular Modeling*, **2018**, 24, 209	2	19
580	Formation of a bi-rhodium boron tube RhB and its great CO capture ability. *Physical Chemistry Chemical Physics*, **2018**, 20, 26072-26082	3.6	11
579	The electronic structure and stability of germanium tubes GeH and GeH. *Physical Chemistry Chemical Physics*, **2018**, 20, 23467-23479	3.6	5
578	Origin of the bright photoluminescence of few-atom silver clusters confined in LTA zeolites. *Science* , **2018**, 361, 686-690	33.3	83
577	Competitive Molecular and Dissociative Hydrogen Chemisorption on Size Selected Doubly Rhodium Doped Aluminum Clusters. *Topics in Catalysis*, **2018**, 61, 62-70	2.3	15
576	Binding affinity of the L-742,001 inhibitor to the endonuclease domain of A/H1N1/PA influenza virus variants: Molecular simulation approaches. *Chemical Physics*, **2018**, 500, 26-36	2.3	5
575	Geometric Structures and Magnetic Interactions in Small Chromium Oxide Clusters. *Journal of Physical Chemistry C*, **2018**, 122, 27640-27647	3.8	6
574	Boron and Nitrogen Co-doped Graphene Used As Counter Electrode for Iodine Reduction in Dye-Sensitized Solar Cells. *Journal of Physical Chemistry C*, **2018**, 122, 26385-26392	3.8	21
573	Structures and magnetic properties of small [Formula: see text] and Co Cr (n = 3-5) clusters. *Journal of Physics Condensed Matter*, **2018**, 30, 474002	1.8	2

572	Effects of the terminal donor unit in dyes with D-D-π-A architecture on the regeneration mechanism in DSSCs: a computational study. *Physical Chemistry Chemical Physics*, **2018**, 20, 23564-23577	3.6	10
571	Multisite occupation of divalent dopants in barium and strontium titanates. *Journal of Physics and Chemistry of Solids*, **2018**, 121, 151-156	3.9	10
570	Mechanistic Study on Water Splitting Reactions by Small Silicon Clusters SiX, X = Si, Be, Mg, Ca. *Journal of Physical Chemistry A*, **2018**, 122, 5132-5141	2.8	3
569	Boron Teetotum: Metallic [Ti(BC N)] and Bimetallic [Ti(BC N)] Nine-Membered Heterocycles with x + y = 3 and -1 □q □3. *Journal of Physical Chemistry A*, **2018**, 122, 6196-6205	2.8	7
568	Theoretical Study of Silicon Monoxide Reactions with Ammonia and Methane. *Journal of Physical Chemistry A*, **2017**, 121, 1032-1040	2.8	0
567	Effects of Charge Transfer on the Adsorption of CO on Small Molybdenum-Doped Platinum Clusters. *Chemistry - A European Journal*, **2017**, 23, 4120-4127	4.8	22
566	Aromatic cage-like B46: existence of the largest decagonal holes in stable atomic clusters. *RSC Advances*, **2017**, 7, 22243-22247	3.7	18
565	Titanium Digermanium: Theoretical Assignment of Electronic Transitions Underlying Its Anion Photoelectron Spectrum. *Journal of Physical Chemistry A*, **2017**, 121, 1940-1949	2.8	14
564	Silicon doped boron clusters: how to make stable ribbons?. *Physical Chemistry Chemical Physics*, **2017**, 19, 14913-14918	3.6	12
563	Structural properties and mechanical stability of lithium-ion based materials. A theoretical study. *Computational Materials Science*, **2017**, 136, 271-279	3.2	6
562	Theoretical Investigation of Metallic Heterofullerenes of Silicon and Germanium Mixed with Phosphorus and Arsenic Atoms M-A8E6, A = Si, Ge; E = P, As; and M = Cr, Mo, W. *Journal of Physical Chemistry A*, **2017**, 121, 5056-5066	2.8	1
561	Structural properties and mechanical stability of monoclinic lithium disilicate. *Physica Status Solidi (B): Basic Research*, **2017**, 254, 1700108	1.3	3
560	Replica exchange molecular dynamics study of the amyloid beta (11-40) trimer penetrating a membrane. *RSC Advances*, **2017**, 7, 7346-7357	3.7	30
559	Structural evolution and bonding of phosphorus-doped silicon clusters SinPm0/+ with n = 1-10, m = 1, 2. *Computational and Theoretical Chemistry*, **2017**, 1107, 115-126	2	5
558	Determination of the absolute binding free energies of HIV-1 protease inhibitors using non-equilibrium molecular dynamics simulations. *Chemical Physics Letters*, **2017**, 676, 12-17	2.5	23
557	Replica exchange molecular dynamics study of the truncated amyloid beta (11-40) trimer in solution. *Physical Chemistry Chemical Physics*, **2017**, 19, 1909-1919	3.6	31
556	4d and 5d bimetal doped tubular silicon clusters SiM with M = Nb, Ta, Mo and W: a bimetallic configuration model. *Physical Chemistry Chemical Physics*, **2017**, 19, 3115-3124	3.6	33
555	Evaluation of the absolute affinity of neuraminidase inhibitor using steered molecular dynamics simulations. *Journal of Molecular Graphics and Modelling*, **2017**, 77, 137-142	2.8	9

554	Comparative Study of Methanol Activation by Different Small Mixed Silicon Clusters SiM with M = H, Li, Na, Cu, and Ag. *ACS Omega*, **2017**, 2, 4563-4574	3.9	3
553	Insights into Geometric and Electronic Structures of VGe Clusters from Anion Photoelectron Spectrum Assignment. *Journal of Physical Chemistry A*, **2017**, 121, 6949-6956	2.8	6
552	Mn@B3N3Si8 +: a stable singlet manganese-doped hetero-atom-mixed silicon fullerene. *Structural Chemistry*, **2017**, 28, 1887-1893	1.8	5
551	On the role of different types of electron in double ring tubular clusters. *Chemical Physics Letters*, **2017**, 685, 377-384	2.5	12
550	Spin-polarized transport properties in some transition metal dithiolene complexes. *Physical Chemistry Chemical Physics*, **2017**, 19, 32536-32543	3.6	4
549	EGCG inhibits the oligomerization of amyloid beta (16-22) hexamer: Theoretical studies. *Journal of Molecular Graphics and Modelling*, **2017**, 76, 1-10	2.8	30
548	Another look at structure of gold clusters Au n from perspective of phenomenological shell model. *Chemical Physics*, **2017**, 493, 140-148	2.3	26
547	Structural assignment of small cationic silver clusters by far-infrared spectroscopy and DFT calculations. *Physical Chemistry Chemical Physics*, **2017**, 19, 19360-19368	3.6	20
546	Structural Evolution, Vibrational Signatures and Energetics of Niobium Clusters from Nb2 to Nb20. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 87-135	0.7	2
545	Transition Metal Doped Boron Clusters: Structure and Bonding of BnM2 Cycles and Tubes. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 199-235	0.7	3
544	Oxygen vacancy generation in rare-earth-doped SrTiO3. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 2197-2203	1.3	9
543	Consequences of Ca multisite occupation for the conducting properties of BaTiO3. *Journal of Solid State Chemistry*, **2016**, 243, 77-82	3.3	4
542	Theoretical study of the interactions between the first transmembrane segment of NS2 protein and a POPC lipid bilayer. *Biophysical Chemistry*, **2016**, 217, 1-7	3.5	5
541	Multiscale simulations on conformational dynamics and membrane interactions of the non-structural 2 (NS2) transmembrane domain. *Biochemical and Biophysical Research Communications*, **2016**, 478, 193-198	3.4	4
540	Silole-Based Nickel Bisdithiolene Complexes: A Theoretical Design for Optoelectronic Applications. *Journal of Physical Chemistry C*, **2016**, 120, 16418-16426	3.8	10
539	Electronic Structure of Neutral and Anionic Scandium Disilicon ScSi Clusters and the Related Anion Photoelectron Spectrum. *Journal of Physical Chemistry A*, **2016**, 120, 9401-9410	2.8	9
538	Structural assignment, and electronic and magnetic properties of lanthanide metal doped silicon heptamers SiM with M = Pr, Gd and Ho. *Physical Chemistry Chemical Physics*, **2016**, 18, 31054-31063	3.6	13
537	Electronic structure of the boron fullerene B14 and its silicon derivatives B13Si(+), B13Si(-) and B12Si2: a rationalization using a cylinder model. *Physical Chemistry Chemical Physics*, **2016**, 18, 17619-26	3.6	8

536	Optical properties of the hydrated charged silver tetramer and silver hexamer encapsulated inside the sodalite cavity of an LTA-type zeolite. *Physical Chemistry Chemical Physics*, **2016**, 18, 18128-36	3.6	17
535	A theoretical study on charge transport of dithiolene nickel complexes. *Physical Chemistry Chemical Physics*, **2016**, 18, 6259-67	3.6	6
534	Aromatic character of planar boron-based clusters revisited by ring current calculations. *Physical Chemistry Chemical Physics*, **2016**, 18, 11919-31	3.6	23
533	Aromatic cages B: unprecedented existence of octagonal holes in boron clusters. *Physical Chemistry Chemical Physics*, **2016**, 18, 11620-3	3.6	15
532	A new chiral boron cluster B44 containing nonagonal holes. *Chemical Communications*, **2016**, 52, 1653-6	5.8	35
531	The potential existence of mixed defect incorporation modes for rare-earth doped cubic BaTiO3. *Physica Status Solidi (B): Basic Research*, **2016**, 253, 733-737	1.3	9
530	Theoretical Study of the SinMgm Clusters and Their Cations: Toward Silicon Nanowires with Magnesium Linkers. *Journal of Physical Chemistry C*, **2016**, 120, 15514-15526	3.8	3
529	Stability and bonding of the multiply coordinated bimetallic boron cycles: B8M22−, B7NM2 and B6C2M2 with M = Sc and Ti. *RSC Advances*, **2016**, 6, 51503-51512	3.7	10
528	Complexes of carbon dioxide with dihalogenated ethylenes: structure, stability and interaction. *RSC Advances*, **2016**, 6, 31401-31409	3.7	7
527	Electronic Structure and Thermochemical Parameters of the Silicon-Doped Boron Clusters BnSi, with n = 8-14, and Their Anions. *Journal of Physical Chemistry A*, **2016**, 120, 3623-33	2.8	15
526	Methanol Activation Catalyzed by Small Earth-Alkali Mixed Silicon Clusters SimMn with M = Be, Mg, Ca and m = 3−4, n = 0−1. *Journal of Physical Chemistry C*, **2016**, 120, 10442-10451	3.8	5
525	Unified reaction pathways for the prebiotic formation of RNA and DNA nucleobases. *Physical Chemistry Chemical Physics*, **2016**, 18, 20177-88	3.6	23
524	Fast and accurate determination of the relative binding affinities of small compounds to HIV-1 protease using non-equilibrium work. *Journal of Computational Chemistry*, **2016**, 37, 2734-2742	3.5	45
523	Theoretical Study of Small Scandium-Doped Silver Clusters ScAg with n = 1-7: Aromatic Feature. *Journal of Physical Chemistry A*, **2016**, 120, 7964-7972	2.8	8
522	Structure Dependent Magnetic Coupling in Cobalt-Doped Silicon Clusters. *Journal of Physical Chemistry C*, **2016**, 120, 19454-19460	3.8	10
521	Correction: Electronic structure of the boron fullerene B and its silicon derivatives BSi, BSi and BSi: a rationalization using a cylinder model. *Physical Chemistry Chemical Physics*, **2016**, 18, 22732	3.6	1
520	Comment on "B38: an all-boron fullerene analogue" by J. Lv, Y. Wang, L. Zhu and Y. Ma, Nanoscale, 2014, 6, 11692. *Nanoscale*, **2015**, 7, 3316-7	7.7	29
519	Design of novel tetra-hetero[8]circulenes: a theoretical study of electronic structure and charge transport characteristics. *RSC Advances*, **2015**, 5, 24167-24174	3.7	12

518	Bonding and singlet-triplet gap of silicon trimer: effects of protonation and attachment of alkali metal cations. *Journal of Computational Chemistry*, **2015**, 36, 805-15	3.5	12
517	Nature of the interaction between rare gas atoms and transition metal doped silicon clusters: the role of shielding effects. *Physical Chemistry Chemical Physics*, **2015**, 17, 17584-91	3.6	10
516	Radical Pathways for the Prebiotic Formation of Pyrimidine Bases from Formamide. *Journal of Physical Chemistry A*, **2015**, 119, 8871-83	2.8	27
515	Decomposition pathways of formamide in the presence of vanadium and titanium monoxides. *Physical Chemistry Chemical Physics*, **2015**, 17, 16927-36	3.6	5
514	Electronic structure and photoelectron spectra of Bn with n = 26-29: an overview of structural characteristics and growth mechanism of boron clusters. *Physical Chemistry Chemical Physics*, **2015**, 17, 13672-9	3.6	46
513	The B32 cluster has the most stable bowl structure with a remarkable heptagonal hole. *Chemical Communications*, **2015**, 51, 7677-80	5.8	35
512	Acetylene as an essential building block for prebiotic formation of pyrimidine bases on Titan. *Physical Chemistry Chemical Physics*, **2015**, 17, 24294-303	3.6	10
511	Fullerene-like boron clusters stabilized by an endohedrally doped iron atom: B(n)Fe with n = 14, 16, 18 and 20. *Physical Chemistry Chemical Physics*, **2015**, 17, 3000-3	3.6	64
510	Mn2@Si15: the smallest triple ring tubular silicon cluster. *Physical Chemistry Chemical Physics*, **2015**, 17, 17566-70	3.6	30
509	Effects of bimetallic doping on small cyclic and tubular boron clusters: B7M2 and B14M2 structures with M = Fe, Co. *Physical Chemistry Chemical Physics*, **2015**, 17, 17335-45	3.6	17
508	Structures, Thermochemical Properties, and Bonding of Mixed Alkaline-Earth-Metal Silicon Trimers Si3M(+/0/-) with M = Be, Mg, Ca. *Journal of Physical Chemistry A*, **2015**, 119, 6493-503	2.8	4
507	Comment on "Computational Study on the Vinyl Azide Decomposition". *Journal of Physical Chemistry A*, **2015**, 119, 12906-7	2.8	7
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