Minh Tho Nguyen

List of Publications by Year
in descending order

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670	15,693	28274	66911
papers	citations	55 h-index	78 g-index

694	694	694	8805
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Boroles. , 2022, , 833-873.		2
2	A Cluster Model for Interpretation of Surface-Enhanced Raman Scattering of Organic Compounds Interacting with Silver Nanoparticles. , 2022, , 255-285.		2
3	Strontium stannate as an alternative anode for Na- and K-Ion batteries: A theoretical study. Journal of Physics and Chemistry of Solids, 2022, 162, 110505.	4.0	6
4	Growth pattern of doubly metal doped silicon clusters M2Sin with M2Â=ÂMo2, Nb2, Ta2, W2, NbMo, TaW and nÂ=Â11â€“18. Formation of fused cages M2Si18. Chemical Physics Letters, 2022, 787, 139229.	2.6	5
5	Unexpected structures of the Au₁₇ gold cluster: the stars are shining. Chemical Communications, 2022, 58, 5785-5788.	4.1	7
6	Evolution of Vibrational Spectra in the Manganeseâ€“Silicon Clusters Mn₂Si_n, n = 10, 12, and 13, and Cationic [Mn₂Si₁₃]⁺. Journal of Physical Chemistry A, 2022, 126, 1617-1626.	2.5	7
7	First-row transition metal doped germanium clusters Ge₁₆M: some remarkable superhalogens. RSC Advances, 2022, 12, 13487-13499.	3.6	2
8	Boron Silicon B₂Si₃^qand B₃Si₂^pClusters: The Smallest Aromatic Ribbons. Journal of Physical Chemistry A, 2022, 126, 3101-3109.	2.5	2
9	Pristine and alkali and alkaline earth metals encapsulated B₃₆N₃₆ nanoclusters as prospective delivery agents and detectors for 5â€fluorouracil anticancer drug. Applied Organometallic Chemistry, 2022, 36, .	3.5	22
10	Unravelling the alkali transport properties in nanocrystalline A₃OX (A = Li, Na, X = Cl, Br) solid state electrolytes. A theoretical prediction. RSC Advances, 2022, 12, 20029-20036.	3.6	9
11	Insights into adsorptive interactions between antibiotic molecules and rutile-TiO2 (110) surface. Surface Science, 2021, 703, 121723.	1.9	6
12	Structure, stability and bonding of the leapfrog B 24 0 ,Â±1,Â±2. Journal of Computational Chemistry, 2021, 42, 72-80.	3.3	4
13	Enhanced Li-ion transport in divalent metal-doped Li₂SnO₃. Dalton Transactions, 2021, 50, 3020-3026.	3.3	6
14	An octacoordinated Nb atom in the NbAl₈H₈⁺ cluster. Chemical Communications, 2021, 57, 9518-9521.	4.1	5
15	Comment on â€˜Structural characterization, reactivity and vibrational properties of silver clusters: a new global minimum for Ag₁₆â€™ by P. L. RodrÃguez-Kessler, A. R. RodrÃguez-DomÃnguez, D. MacLeod Carey and A. MuÃ±oz-Castro, Phys. Chem. Chem. Phys., 2020, 22, 27255, DOI: D0CP04018F. Physical Chemistry Chemical Physics, 2021, 23, 12900-12903.	2.8	3
16	Gold nanoclusters as prospective carriers and detectors of pramipexole. RSC Advances, 2021, 11, 16619-16632.	3.6	20
17	Another look at the structure of the (H2O)nâ€¢Ö¾ system: water anion vs. hydrated electron. Structural Chemistry, 2021, 32, 655-665.	2.0	2
18	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.	2.5	12

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19	A theoretical design of bipolar host materials for blue phosphorescent OLED. Journal of Molecular Graphics and Modelling, 2021, 105, 107845.	2.4	3
20	Strontium Stannate as an Alternative Anode Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2021, 125, 14947-14956.	3.1	9
21	Another look at energetically quasiâ€degenerate structures of the gold cluster Au 27 q with qÂ=Â1, 0, â¯1. Journal of Computational Chemistry, 2021, 42, 2145-2153.	3.3	3
22	Design of fused bithiophene systems containing silole and five-membered heterocycles for optoelectronic materials. Chemical Physics Letters, 2021, 784, 139093.	2.6	2
23	Adsorption/Desorption Behaviors and SERS Chemical Enhancement of 6-Mercaptopurine on a Nanostructured Gold Surface: The Au20 Cluster Model. Molecules, 2021, 26, 5422.	3.8	8
24	SERS Chemical Enhancement of 2,4,5-Trichlorophenoxyacetic Acid Adsorbed on Silver Substrate. Journal of Physical Chemistry A, 2021, 125, 8529-8541.	2.5	14
25	The binary boron lithium clusters B₁₂Li_n with n = 1â€“14: in search for hydrogen storage materials. Physical Chemistry Chemical Physics, 2021, 23, 24866-24877.	2.8	7
26	Theoretical Aspects of Nonconventional Hydrogen Bonds in the Complexes of Aldehydes and Hydrogen Chalcogenides. Journal of Physical Chemistry A, 2021, 125, 10291-10302.	2.5	2
27	The binary aluminum scandium clusters Al_xSc_y with x + y = 13: when is the icosahedron retained?. RSC Advances, 2021, 11, 40072-40084.	3.6	2
28	The lowest-energy structure of the gold cluster Au₁₀: planar vs. nonplanar?. Physical Chemistry Chemical Physics, 2021, 24, 42-47.	2.8	9
29	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.	2.0	2
30	Structures and Magnetism of Cationic Chromiumâ€“Manganese Bimetallic Oxide Clusters. Journal of Physical Chemistry C, 2020, 124, 2598-2608.	3.1	2
31	Theoretical study on the interaction of iodide electrolyte/organic dye with the TiO₂ surface in dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2020, 22, 26410-26418.	2.8	7
32	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.	2.8	1
33	Structural Evolution and Stability Trend of Small-Sized Gold Clusters Au_n (n = 20â€“30). Journal of Physical Chemistry A, 2020, 124, 1289-1299.	2.5	23
34	Structural, electronic, and optical properties of some new dithienosilole derivatives. Structural Chemistry, 2020, 31, 2215-2225.	2.0	1
35	Substituent Effects on the Nâ€“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.	3.5	3
36	Boosting Li-Ion Transport in Transition-Metal-Doped Li₂SnO₃. Inorganic Chemistry, 2020, 59, 11841-11846.	4.0	15

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37	SERS Spectra of the Pesticide Chlorpyrifos Adsorbed on Silver Nanosurface: The Ag₂₀ Cluster Model. Journal of Physical Chemistry C, 2020, 124, 21702-21716.	3.1	31
38	Structure and Stability of a Trefoil Leaf Motif of Metal-Doped Silicon and Germanium Clusters: M₃@E₂₀ with E = Si and Ge and M = Fe, Ru, and Os. Journal of Physical Chemistry A, 2020, 124, 8488-8495.	2.5	0
39	Autocatalysis in Formose Reaction and Formation of RNA Nucleosides. Journal of Physical Chemistry B, 2020, 124, 11324-11336.	2.6	10
40	Influence of Fluorination on Energetic Parameters of Silole, Phosphole, Thiophene, Oligomers of Silole and Related Acenes. Journal of Fluorine Chemistry, 2020, 240, 109665.	1.7	3
41	Interplay between Ïƒ Holes, AnionÂ·Â·Â·Hâ€“C, and Cationâ‹¯Ï€ Interactions in Dibromo[2,2]paracyclophane Complexes. Journal of Physical Chemistry A, 2020, 124, 4379-4389.	2.5	5
42	Molecular structure, IR, Raman and UVâ€“VIS spectra of 2-cyanothiophene and 3-cyanothiophene: A comparative quantum chemical investigation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118393.	3.9	6
43	The teetotum cluster Li₂FeB₁₄and its possible use for constructing boron nanowires. Physical Chemistry Chemical Physics, 2020, 22, 15013-15021.	2.8	3
44	A remarkable mixture of germanium with phosphorus and arsenic atoms making stable pentagonal hetero-prisms [M@Ge5E5]+, E = P, As and M = Fe, Ru, Os. RSC Advances, 2020, 10, 19781-19789.	3.6	3
45	Optoelectronic properties of heptacene, its fluorinated derivatives and silole, thiophene analogues. Materials Today Communications, 2020, 24, 101054.	1.9	0
46	Electronic Structure and Properties of Silicon-Doped Boron Clusters B_nSi withn= 15â€“24 and Their Anions. Journal of Physical Chemistry C, 2020, 124, 6770-6783.	3.1	9
47	Theoretical Study of a Class of Organic D-Ï€-A Dyes for Polymer Solar Cells: Influence of Various Ï€-Spacers. Crystals, 2020, 10, 163.	2.2	6
48	Hydrogen Adsorption and Dissociation on Al_nRh₂⁺ (n = 1 to 9) Clusters: Steric and Coordination Effects. Journal of Physical Chemistry C, 2020, 124, 7624-7633.	3.1	12
49	Structures, stabilities and aromatic properties of endohedrally transition metal doped boron clusters M@B₂₂, M = Sc and Ti: a theoretical study. Physical Chemistry Chemical Physics, 2020, 22, 8077-8087.	2.8	8
50	Na- and K-Doped Li₂SiO₃ as an Alternative Solid Electrolyte for Solid-State Lithium Batteries. Journal of Physical Chemistry C, 2020, 124, 4982-4988.	3.1	12
51	Impact of the Astaxanthin, Betanin, and EGCG Compounds on Small Oligomers of Amyloid Aî²₄₀ Peptide. Journal of Chemical Information and Modeling, 2020, 60, 1399-1408.	5.4	17
52	Silole and selenophene-based D-Ï€-A dyes in dye-sensitized solar cells: Insights from optoelectronic and regeneration properties. Dyes and Pigments, 2020, 176, 108243.	3.7	6
53	A molecular level insight into adsorption of Î²-lactam antibiotics on vermiculite surface. Surface Science, 2020, 695, 121588.	1.9	8
54	Elucidating the binding mechanism of thioneâ€containing mercaptopurine and thioguanine drugs to small gold clusters. Journal of Computational Chemistry, 2020, 41, 1748-1758.	3.3	19

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55	Advances in Synthesis of Ï€-Extended Benzosilole Derivatives and Their Analogs. Molecules, 2020, 25, 548.	3.8	17
56	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.	2.6	3
57	Influence of Oxygenâ€“Sulfur Exchange on the Structural, Electronic, and Stability Properties of Alkali Hexastannates. Journal of Physical Chemistry C, 2019, 123, 24375-24382.	3.1	6
58	B_xGe₁₂^{0/+} Clusters with x = 1â€“4: Germanium Tubes Stabilized by Three and Four Boron Dopants. Journal of Physical Chemistry C, 2019, 123, 24676-24684.	3.1	3
59	Lithium- and sodium-ion transport properties of Li2Ti6O13, Na2Ti6O13 and Li2Sn6O13. Journal of Solid State Chemistry, 2019, 279, 120930.	2.9	11
60	Formation of the M₂B₁₈^q Teetotum Boron Clusters with 4d and 5d Transition Metals M = Rh, Pd, Ir, and Pt. Journal of Physical Chemistry A, 2019, 123, 8170-8178.	2.5	10
61	Structure, stability, absorption spectra and aromaticity of the singly and doubly silicon doped aluminum clusters Al_nSi_m^{0/+} with n = 3â€“16 and m = 1, 2. RSC Advances, 2019, 9, 27208-27223.	3.6	5
62	Valence bonds in planar and quasi-planar boron disks. Physical Chemistry Chemical Physics, 2019, 21, 729-735.	2.8	5
63	Remarkable shifts of C sp2 â€H and Oâ€H stretching frequencies and stability of complexes of formic acid with formaldehydes and thioformaldehydes. Journal of Computational Chemistry, 2019, 40, 1387-1400.	3.3	10
64	Hydrogen Chemisorption on Doubly Vanadium Doped Aluminum Clusters. Zeitschrift Fur Physikalische Chemie, 2019, 233, 799-812.	2.8	8
65	A theoretical approach to the role of different types of electrons in planar elongated boron clusters. Physical Chemistry Chemical Physics, 2019, 21, 13030-13039.	2.8	11
66	Comment on â€œTheoretical Investigations on Geometrical and Electronic Structures of Silver Clustersâ€• Journal of Computational Chemistry, 2019, 40, 1990-1993.	3.3	3
67	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.	2.6	3
68	Implications of Oxygenâ€“Sulfur Exchange on Structural, Electronic Properties, and Stability of Alkaliâ€Metal Hexatitanates. Physica Status Solidi (B): Basic Research, 2019, 256, 1800568.	1.5	7
69	Impressive capacity of the B7â^' and V2B7 clusters for CO2 capture. Chemical Physics Letters, 2019, 728, 186-194.	2.6	6
70	A model study on the mechanism and kinetics for the dissociation of water anion. International Journal of Chemical Kinetics, 2019, 51, 610-617.	1.6	2
71	Formation of the quasi-planar B₅₀ boron cluster: topological path from B₁₀ and disk aromaticity. Physical Chemistry Chemical Physics, 2019, 21, 7039-7044.	2.8	17
72	Effects of single and double nickel doping on boron clusters: stabilization of tubular structures in B_nNi_m,n= 2â€“22,m= 1, 2. Physical Chemistry Chemical Physics, 2019, 21, 8365-8375.	2.8	26

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73	The scandium doped boron cluster B₂₇Sc₂⁺: a fruit can-like structure. Physical Chemistry Chemical Physics, 2019, 21, 8933-8939.	2.8	14
74	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.	3.1	6
75	Geometry and bonding of small binary boron-aluminum clusters BnAln (nâ€¯=â€¯1â€“7): Electron donation and interlocking aromaticity. Chemical Physics Letters, 2019, 714, 87-93.	2.6	6
76	Insights into the cooperativity between multiple interactions of dimethyl sulfoxide with carbon dioxide and water. Journal of Computational Chemistry, 2019, 40, 464-474.	3.3	11
77	B₃@Si₁₂⁺: strong stabilizing effects of a triatomic cyclic boron unit on tubular silicon clusters. Physical Chemistry Chemical Physics, 2018, 20, 7588-7592.	2.8	12
78	Cover Image, Volume 86, Issue 4. Proteins: Structure, Function and Bioinformatics, 2018, 86, C1.	2.6	0
79	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.	2.5	9
80	Lithium Hexastannate: A Potential Material for Energy Storage. Physica Status Solidi (B): Basic Research, 2018, 255, 1700669.	1.5	16
81	Propafenone effects on the stable structures of AÎ²16-22 system. Chemical Physics Letters, 2018, 696, 55-60.	2.6	6
82	Molecular details of spontaneous insertion and interaction of HCV nonâ€structure 3 protease protein domain with PIP2â€containing membrane. Proteins: Structure, Function and Bioinformatics, 2018, 86, 423-433.	2.6	1
83	Aromaticity of Some Metal Clusters: A Different View from Magnetic Ring Current. Journal of Physical Chemistry A, 2018, 122, 1378-1391.	2.5	7
84	A theoretical design of some silole-based dibenzothiophene-S,S-dioxide semiconducting compounds for red phosphorescence. Organic Electronics, 2018, 54, 270-276.	2.6	6
85	Insight into the adsorption of chloramphenicol on a vermiculite surface. Chemical Physics Letters, 2018, 699, 107-114.	2.6	16
86	Competitive Molecular and Dissociative Hydrogen Chemisorption on Size Selected Doubly Rhodium Doped Aluminum Clusters. Topics in Catalysis, 2018, 61, 62-70.	2.8	20
87	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.	1.9	7
88	Geometric Structures and Magnetic Interactions in Small Chromium Oxide Clusters. Journal of Physical Chemistry C, 2018, 122, 27640-27647.	3.1	9
89	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.	3.1	31
90	Structures and magnetic properties of small ${{\rm Co}_{n}^{+}}$ and Co_{nâ‾1}Cr⁺ (nâ€‰â€‰=â€‰â€‰3â€“5) clusters. Journal of Physics Condensed Matter, 2018, 30, 474002.	1.8	11

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91	Effects of the terminal donor unit in dyes with Dâ€“Dâ€“Ïâ€“A architecture on the regeneration mechanism in DSSCs: a computational study. Physical Chemistry Chemical Physics, 2018, 20, 23564-23577.	2.8	15
92	Multisite occupation of divalent dopants in barium and strontium titanates. Journal of Physics and Chemistry of Solids, 2018, 121, 151-156.	4.0	12
93	Mechanistic Study on Water Splitting Reactions by Small Silicon Clusters Si₃X, X = Si, Be, Mg, Ca. Journal of Physical Chemistry A, 2018, 122, 5132-5141.	2.5	4
94	Boron Teetotum: Metallic [Ti(B₆C_xN_y)]^q and Bimetallic [Ti₂(B₆C_xN_y)]^q Nine-Membered Heterocycles with x + y = 3 and â˜'1 â‰¤ q â‰¤ 3. Journal of Physical Chemistry A, 2018, 122, 6196-6205.	2.5	8
95	Another Look at Photoelectron Spectra of the Anion Cr₂O₂^{â€“}: Multireference Character and Energetic Degeneracy. Journal of Chemical Theory and Computation, 2018, 14, 4833-4843.	5.3	5
96	Size Dependent H₂ Adsorption on Al_nRh⁺ (n = 1â€“12) Clusters. Journal of Physical Chemistry C, 2018, 122, 18247-18255.	3.1	26
97	Elucidation of the molecular and electronic structures of some magic silver clusters Agn (nâ€‰=â€‰8, 18,) Tj ETQq1 1 0.784314 rgBT	1.8	23
98	Formation of a bi-rhodium boron tube Rh₂B₁₈ and its great CO₂ capture ability. Physical Chemistry Chemical Physics, 2018, 20, 26072-26082.	2.8	11
99	The electronic structure and stability of germanium tubes Ge₃₀H₁₂ and Ge₃₃H₁₂. Physical Chemistry Chemical Physics, 2018, 20, 23467-23479.	2.8	6
100	Origin of the bright photoluminescence of few-atom silver clusters confined in LTA zeolites. Science, 2018, 361, 686-690.	12.6	134
101	Theoretical Study of Silicon Monoxide Reactions with Ammonia and Methane. Journal of Physical Chemistry A, 2017, 121, 1032-1040.	2.5	2
102	Effects of Charge Transfer on the Adsorption of CO on Small Molybdenumâ€Doped Platinum Clusters. Chemistry - A European Journal, 2017, 23, 4120-4127.	3.3	27
103	Aromatic cage-like B₄₆: existence of the largest decagonal holes in stable atomic clusters. RSC Advances, 2017, 7, 22243-22247.	3.6	23
104	Titanium Digermanium: Theoretical Assignment of Electronic Transitions Underlying Its Anion Photoelectron Spectrum. Journal of Physical Chemistry A, 2017, 121, 1940-1949.	2.5	16
105	Silicon doped boron clusters: how to make stable ribbons?. Physical Chemistry Chemical Physics, 2017, 19, 14913-14918.	2.8	18
106	Structural properties and mechanical stability of lithium-ion based materials. A theoretical study. Computational Materials Science, 2017, 136, 271-279.	3.0	10
107	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.	2.5	1
108	Structural properties and mechanical stability of monoclinic lithium disilicate. Physica Status Solidi (B): Basic Research, 2017, 254, 1700108.	1.5	6

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109	Replica exchange molecular dynamics study of the amyloid beta (11â€“40) trimer penetrating a membrane. RSC Advances, 2017, 7, 7346-7357.	3.6	38
110	Structural evolution and bonding of phosphorus-doped silicon clusters SinPmâ^'/0/+ with n = 1â€“10, m = 1, 2. Computational and Theoretical Chemistry, 2017, 1107, 115-126.	2.5	6
111	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.	2.6	27
112	Replica exchange molecular dynamics study of the truncated amyloid beta (11â€“40) trimer in solution. Physical Chemistry Chemical Physics, 2017, 19, 1909-1919.	2.8	36
113	4d and 5d bimetal doped tubular silicon clusters Si₁₂M₂ with M = Nb, Ta, Mo and W: a bimetallic configuration model. Physical Chemistry Chemical Physics, 2017, 19, 3115-3124.	2.8	36
114	Evaluation of the absolute affinity of neuraminidase inhibitor using steered molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2017, 77, 137-142.	2.4	12
115	Comparative Study of Methanol Activation by Different Small Mixed Silicon Clusters Si₂M with M = H, Li, Na, Cu, and Ag. ACS Omega, 2017, 2, 4563-4574.	3.5	4
116	Insights into Geometric and Electronic Structures of VGe₃^{â€“/0} Clusters from Anion Photoelectron Spectrum Assignment. Journal of Physical Chemistry A, 2017, 121, 6949-6956.	2.5	7
117	Mn@B3N3Si8 +: a stable singlet manganese-doped hetero-atom-mixed silicon fullerene. Structural Chemistry, 2017, 28, 1887-1893.	2.0	5
118	On the role of different types of electron in double ring tubular clusters. Chemical Physics Letters, 2017, 685, 377-384.	2.6	13
119	Spin-polarized transport properties in some transition metal dithiolene complexes. Physical Chemistry Chemical Physics, 2017, 19, 32536-32543.	2.8	4
120	EGCG inhibits the oligomerization of amyloid beta (16-22) hexamer: Theoretical studies. Journal of Molecular Graphics and Modelling, 2017, 76, 1-10.	2.4	38
121	Another look at structure of gold clusters Au n from perspective of phenomenological shell model. Chemical Physics, 2017, 493, 140-148.	1.9	40
122	Structural assignment of small cationic silver clusters by far-infrared spectroscopy and DFT calculations. Physical Chemistry Chemical Physics, 2017, 19, 19360-19368.	2.8	31
123	Structural Evolution, Vibrational Signatures and Energetics of Niobium Clusters from Nb2 to Nb20. Challenges and Advances in Computational Chemistry and Physics, 2017, , 87-135.	0.6	2
124	Transition Metal Doped Boron Clusters: Structure and Bonding of BnM2 Cycles and Tubes. Challenges and Advances in Computational Chemistry and Physics, 2017, , 199-235.	0.6	3
125	The potential existence of mixed defect incorporation modes for rare-earth doped cubic BaTiO₃. Physica Status Solidi (B): Basic Research, 2016, 253, 733-737.	1.5	10
126	Theoretical Study of the SinMgm Clusters and Their Cations: Toward Silicon Nanowires with Magnesium Linkers. Journal of Physical Chemistry C, 2016, 120, 15514-15526.	3.1	4

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127	Stability and bonding of the multiply coordinated bimetallic boron cycles: B₈M₂^{2â^'}, B₇NM₂and B₆C₂M₂with M = Sc and Ti. RSC Advances, 2016, 6, 51503-51512.	3.6	12
128	Complexes of carbon dioxide with dihalogenated ethylenes: structure, stability and interaction. RSC Advances, 2016, 6, 31401-31409.	3.6	7
129	Electronic Structure and Thermochemical Parameters of the Silicon-Doped Boron Clusters B_nSi, with n = 8â€“14, and Their Anions. Journal of Physical Chemistry A, 2016, 120, 3623-3633.	2.5	21
130	Methanol Activation Catalyzed by Small Earth-Alkali Mixed Silicon Clusters Si_{mâ€“n}M_n with M = Be, Mg, Ca and m = 3â€“4, n = 0â€“1. Journal of Physical Chemistry C, 2016, 120, 10442-10451.	3.1	6
131	Unified reaction pathways for the prebiotic formation of RNA and DNA nucleobases. Physical Chemistry Chemical Physics, 2016, 18, 20177-20188.	2.8	34
132	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.	3.3	70
133	Theoretical Study of Small Scandium-Doped Silver Clusters ScAgn with n = 1â€“7: Ïƒ-Aromatic Feature. Journal of Physical Chemistry A, 2016, 120, 7964-7972.	2.5	12
134	Structure Dependent Magnetic Coupling in Cobalt-Doped Silicon Clusters. Journal of Physical Chemistry C, 2016, 120, 19454-19460.	3.1	15
135	Correction: Electronic structure of the boron fullerene B14 and its silicon derivatives B13Si+, B13Siâ^' and B12Si2: a rationalization using a cylinder model. Physical Chemistry Chemical Physics, 2016, 18, 22732-22732.	2.8	1
136	Oxygen vacancy generation in rareâ€earthâ€doped SrTiO₃. Physica Status Solidi (B): Basic Research, 2016, 253, 2197-2203.	1.5	11
137	Consequences of Ca multisite occupation for the conducting properties of BaTiO3. Journal of Solid State Chemistry, 2016, 243, 77-82.	2.9	8
138	Theoretical study of the interactions between the first transmembrane segment of NS2 protein and a POPC lipid bilayer. Biophysical Chemistry, 2016, 217, 1-7.	2.8	8
139	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.	2.1	4
140	Silole-Based Nickel Bisdithiolene Complexes: A Theoretical Design for Optoelectronic Applications. Journal of Physical Chemistry C, 2016, 120, 16418-16426.	3.1	13
141	Electronic Structure of Neutral and Anionic Scandium Disilicon ScSi₂^{â€“/0} Clusters and the Related Anion Photoelectron Spectrum. Journal of Physical Chemistry A, 2016, 120, 9401-9410.	2.5	9
142	Structural assignment, and electronic and magnetic properties of lanthanide metal doped silicon heptamers Si₇M^{0/â^'} with M = Pr, Gd and Ho. Physical Chemistry Chemical Physics, 2016, 18, 31054-31063.	2.8	16
143	Electronic structure of the boron fullerene B₁₄ and its silicon derivatives B₁₃Si⁺, B₁₃Si^{â^'} and B₁₂Si₂: a rationalization using a cylinder model. Physical Chemistry Chemical Physics, 2016, 18, 17619-17626.	2.8	11
144	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, 18128-18136.	2.8	23

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145	A theoretical study on charge transport of dithiolene nickel complexes. Physical Chemistry Chemical Physics, 2016, 18, 6259-6267.	2.8	7
146	Aromatic character of planar boron-based clusters revisited by ring current calculations. Physical Chemistry Chemical Physics, 2016, 18, 11919-11931.	2.8	31
147	Aromatic cages B0/+42: unprecedented existence of octagonal holes in boron clusters. Physical Chemistry Chemical Physics, 2016, 18, 11620-11623.	2.8	16
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