Nguyen Minh Tam

List of Publications by Year in Descending Order

60 papers	855 citations	17 h-index	27 g-index
71 ext. papers	1,009 ext. citations	3.2 avg, IF	4.65 L-index

#	Paper	IF	Citations
60	Unbinding ligands from SARS-CoV-2 Mpro via umbrella sampling simulations.. *Royal Society Open Science*, **2022**, 9, 211480	3.3	0
59	DFT investigation of Au9M2+ nanoclusters (M = Sc-Ni): The magnetic superatomic behavior of Au9Cr2+. *Chemical Physics Letters*, **2022**, 793, 139451	2.5	0
58	Improving ligand-ranking of AutoDock Vina by changing the empirical parameters. *Journal of Computational Chemistry*, **2022**, 43, 160-169	3.5	6
57	In silico screening of potential □secretase (BACE1) inhibitors from VIETHERB database.. *Journal of Molecular Modeling*, **2022**, 28, 60	2	
56	First-row transition metal doped germanium clusters GeM: some remarkable superhalogens.. *RSC Advances*, **2022**, 12, 13487-13499	3.7	0
55	Searching and designing potential inhibitors for SARS-CoV-2 Mpro from natural sources using atomistic and deep-learning calculations.. *RSC Advances*, **2021**, 11, 38495-38504	3.7	2
54	The binary aluminum scandium clusters Al Sc with + = 13: when is the icosahedron retained?. *RSC Advances*, **2021**, 11, 40072-40084	3.7	0
53	Designs, Synthesis, Docking Studies, and Biological Evaluation of Novel Berberine Derivatives Targeting Zika Virus. *Journal of Chemistry*, **2021**, 2021, 1-10	2.3	1
52	Benchmark of Popular Free Energy Approaches Revealing the Inhibitors Binding to SARS-CoV-2 Mpro. *Journal of Chemical Information and Modeling*, **2021**, 61, 2302-2312	6.1	28
51	The radical scavenging activity of abietane diterpenoids: Theoretical insights. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107892	2.8	2
50	A theoretical design of bipolar host materials for blue phosphorescent OLED. *Journal of Molecular Graphics and Modelling*, **2021**, 105, 107845	2.8	1
49	Binding of inhibitors to the monomeric and dimeric SARS-CoV-2 Mpro.. *RSC Advances*, **2021**, 11, 2926-2934	3.7	13
48	Computational estimation of potential inhibitors from known drugs against the main protease of SARS-CoV-2.. *RSC Advances*, **2021**, 11, 17478-17486	3.7	9
47	Systematic Investigation of the Structure, Stability, and Spin Magnetic Moment of CrM Clusters (M = Cu, Ag, Au, and = 2-20) by DFT Calculations. *ACS Omega*, **2021**, 6, 20341-20350	3.9	1
46	Mechanistic and kinetic studies of the radical scavenging activity of natural abietanes: A theoretical insight. *Chemical Physics Letters*, **2021**, 777, 138737	2.5	0
45	Marine derivatives prevent MUS81 studies. *Royal Society Open Science*, **2021**, 8, 210974	3.3	0
44	Potential inhibitors for SARS-CoV-2 Mpro from marine compounds.. *RSC Advances*, **2021**, 11, 22206-22213	3.7	5

43	A thermodynamic and kinetic study of the antioxidant activity of natural hydroanthraquinones.. *RSC Advances*, **2020**, 10, 20089-20097	3.7	14
42	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
41	Interaction of carbon monoxide with doped metal clusters. *CrystEngComm*, **2020**, 22, 4807-4815	3.3	5
40	The radical scavenging activity of natural ramalin: A mechanistic and kinetic study. *Chemical Physics Letters*, **2020**, 739, 137004	2.5	11
39	Substitution effects on the antiradical activity of hydralazine: a DFT analysis. *New Journal of Chemistry*, **2020**, 44, 16577-16583	3.6	8
38	The antioxidant activity of natural diterpenes: theoretical insights.. *RSC Advances*, **2020**, 10, 14937-14943	3.7	15
37	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
36	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
35	Geometry and bonding of small binary boron-aluminum clusters BnAln (n = 17): Electron donation and interlocking aromaticity. *Chemical Physics Letters*, **2019**, 714, 87-93	2.5	3
34	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
33	Influence of various force fields in estimating the binding affinity of acetylcholinesterase inhibitors using fast pulling of ligand scheme. *Chemical Physics Letters*, **2018**, 701, 65-71	2.5	9
32	Ultimate Manipulation of Magnetic Moments in the Golden Tetrahedron Au20 with a Substitutional 3d Impurity. *Journal of Physical Chemistry C*, **2018**, 122, 16256-16264	3.8	5
31	Conjugated polymers: A systematic investigation of their electronic and geometric properties using density functional theory and semi-empirical methods. *Synthetic Metals*, **2018**, 246, 128-136	3.6	8
30	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
29	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
28	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
27	A DFT investigation on geometry and chemical bonding of isoelectronic Si8N6V, Si8N6Cr, and Si8N6Mn+ clusters. *Chemical Physics Letters*, **2017**, 685, 410-415	2.5	1
26	AuM (M=Cr, Mn, and Fe) as magnetic copies of the golden pyramid. *Scientific Reports*, **2017**, 7, 16086	4.9	11

25	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
24	A Systematic Investigation on CrCun Clusters with n = 9-16: Noble Gas and Tunable Magnetic Property. *Journal of Physical Chemistry A*, **2016**, 120, 7335-43	2.8	11
23	Structure, magnetism, and dissociation energy of small bimetallic cobalt-chromium oxide cluster cations: A density-functional-theory study. *Chemical Physics Letters*, **2016**, 643, 77-83	2.5	4
22	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
21	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
20	Structure Dependent Magnetic Coupling in Cobalt-Doped Silicon Clusters. *Journal of Physical Chemistry C*, **2016**, 120, 19454-19460	3.8	10
19	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
18	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
17	Mn2@Si15: the smallest triple ring tubular silicon cluster. *Physical Chemistry Chemical Physics*, **2015**, 17, 17566-70	3.6	30
16	Structure assignment, electronic properties, and magnetism quenching of endohedrally doped neutral silicon clusters, Si(n)Co (n = 10-12). *Journal of Physical Chemistry A*, **2014**, 118, 8198-203	2.8	32
15	Planar tetracoordinate carbon stabilized by heavier congener cages: The Si9C and Ge9C clusters. *Chemical Physics Letters*, **2014**, 595-596, 272-276	2.5	17
14	A particle on a hollow cylinder: the triple ring tubular cluster B27(+). *Physical Chemistry Chemical Physics*, **2014**, 16, 19470-8	3.6	45
13	Influence of Cr doping on the stability and structure of small cobalt oxide clusters. *Journal of Chemical Physics*, **2014**, 141, 044311	3.9	14
12	Ring currents in silicon tetramer (Si4, Si42+) and planar tetracoordinate carbon doped cluster Si4C2+: versus aromaticity. *Chemical Physics Letters*, **2014**, 608, 255-263	2.5	19
11	The boron conundrum: Bonding in the bowl B30 and B36, fullerene B40 and triple ring B42 clusters. *Chemical Physics Letters*, **2014**, 608, 295-302	2.5	52
10	The Boron conundrum: the case of cationic clusters ({rm{B}}^{+}_{n}) with n = 2−20. *Highlights in Theoretical Chemistry*, **2014**, 71-85		
9	Structure, thermochemical properties, and growth sequence of aluminum-doped silicon clusters Si(n)Al(m) (n = 1-11, m = 1-2) and their anions. *Journal of Physical Chemistry A*, **2013**, 117, 6867-82	2.8	23
8	Heat of formation and thermochemical parameters of silole. *Chemical Physics Letters*, **2013**, 588, 17-21	2.5	2

7	Heats of formation and thermochemical parameters of small silicon clusters and their ions, Sin+/0/- with n = 2–13. *Chemical Physics Letters*, **2013**, 584, 147-154	2.5	19
6	Structure of boron clusters revisited, Bn with n = 14–20. *Chemical Physics Letters*, **2012**, 530, 71-76	2.5	89
5	Thermochemical Parameters and Growth Mechanism of the Boron-Doped Silicon Clusters, SinBq with n = 1–10 and q = –1, 0, +1. *Journal of Physical Chemistry C*, **2012**, 116, 20086-20098	3.8	36
4	Ionization energies and structures of lithium doped silicon clusters. *Physical Chemistry Chemical Physics*, **2012**, 14, 8542-50	3.6	17
3	Singly and doubly lithium doped silicon clusters: geometrical and electronic structures and ionization energies. *Journal of Chemical Physics*, **2012**, 136, 024301	3.9	16
2	The Boron conundrum: the case of cationic clusters B + n with n = 2–20. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	51
1	Evolution of structures and stabilities of zinc-doped tin clusters SnnZn, n=1–12. Three-dimensional aromaticity of the magic clusters Sn10Zn and Sn12Zn. *Chemical Physics*, **2011**, 388, 1-8	2.3	18