Minh Tho Nguyen

List of Publications by Citations

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	Carboxyl-functionalized task-specific ionic liquids for solubilizing metal oxides. *Inorganic Chemistry*, **2008**, 47, 9987-99	5.1	207
660	Molecular mechanism for H2 release from BH3NH3, including the catalytic role of the Lewis acid BH3. *Journal of Physical Chemistry A*, **2007**, 111, 679-90	2.8	154
659	Polynitrogen compounds. *Coordination Chemistry Reviews*, **2003**, 244, 93-113	23.2	149
658	How Many Water Molecules Are Actively Involved in the Neutral Hydration of Carbon Dioxide?. *Journal of Physical Chemistry A*, **1997**, 101, 7379-7388	2.8	128
657	A unified perspective on the hydrogen atom transfer and proton-coupled electron transfer mechanisms in terms of topographic features of the ground and excited potential energy surfaces as exemplified by the reaction between phenol and radicals. *Journal of the American Chemical Society*, **2008**, 130, 7000-10	16.4	125
656	Computational study of the release of H2 from ammonia borane dimer (BH3NH3)2 and its ion pair isomers. *Journal of Physical Chemistry A*, **2007**, 111, 8844-56	2.8	118
655	Theoretical Study of the Interaction between Thymine and Water. Protonation and Deprotonation Enthalpies and Comparison with Uracil. *Journal of Physical Chemistry A*, **1998**, 102, 6010-6016	2.8	116
654	Unimolecular rearrangements connecting hydroxyethylidene (CH3-C-OH), acetaldehyde (CH3-CH:O), and vinyl alcohol (CH2:CH-OH). *Journal of the American Chemical Society*, **1991**, 113, 6452-6458	16.4	114
653	Theoretical Study of Tautomeric Forms of Uracil. 1. Relative Order of Stabilities and Their Relation to Proton Affinities and Deprotonation Enthalpies. *Journal of Physical Chemistry A*, **2001**, 105, 1288-1295	2.8	110
652	Thermochemistry and electronic structure of small boron clusters (B(n), n = 5-13) and their anions. *Journal of Physical Chemistry A*, **2010**, 114, 994-1007	2.8	102
651	Mechanism of the hydration of carbon dioxide: direct participation of H2O versus microsolvation. *Journal of Physical Chemistry A*, **2008**, 112, 10386-98	2.8	99
650	Theoretical Study of Uracil Tautomers. 2. Interaction with Water. *Journal of Physical Chemistry A*, **2001**, 105, 1934-1943	2.8	99
649	Mechanism of [2 + 1] Cycloadditions of Hydrogen Isocyanide to Alkynes: Molecular Orbital and Density Functional Theory Study. *Journal of the American Chemical Society*, **1999**, 121, 5992-6001	16.4	95
648	Protonation and deprotonation energies of uracil Implications for the uracil–water complex. *Journal of the Chemical Society, Faraday Transactions*, **1998**, 94, 1277-1280		94
647	Another Look at the Mechanism of the Concerted 1,3-Dipolar Cycloaddition of Fulminic Acid to Acetylene. *Journal of Organic Chemistry*, **1999**, 64, 65-69	4.2	92
646	Protonation and Deprotonation Enthalpies of Guanine and Adenine and Implications for the Structure and Energy of Their Complexes with Water:´Comparison with Uracil, Thymine, and Cytosine. *Journal of Physical Chemistry A*, **1999**, 103, 8853-8860	2.8	91
645	Structure of boron clusters revisited, Bn with n = 14–20. *Chemical Physics Letters*, **2012**, 530, 71-76	2.5	89

644	A New Look at the Classical Beckmann Rearrangement: A Strong Case of Active Solvent Effect. *Journal of the American Chemical Society*, **1997**, 119, 2552-2562	16.4	87
643	Potential energy surfaces, product distributions and thermal rate coefficients of the reaction of O(3P) with C2H4(X1Ag): a comprehensive theoretical study. *Journal of Physical Chemistry A*, **2005**, 109, 7489-99	2.8	87
642	Theoretical Study of the Thermal Decomposition of Acetic Acid: Decarboxylation Versus Dehydration. *The Journal of Physical Chemistry*, **1995**, 99, 11883-11888		84
641	Origin of the bright photoluminescence of few-atom silver clusters confined in LTA zeolites. *Science* , **2018**, 361, 686-690	33.3	83
640	A Stochastic Search for the Structures of Small Germanium Clusters and Their Anions: Enhanced Stability by Spherical Aromaticity of the Ge10 and Ge12(2-) Systems. *Journal of Chemical Theory and Computation*, **2011**, 7, 1119-30	6.4	83
639	Density Functional Approach to Regiochemistry, Activation Energy, and Hardness Profile in 1,3-Dipolar Cycloadditions. *Journal of Physical Chemistry A*, **1998**, 102, 6181-6185	2.8	77
638	Disk aromaticity of the planar and fluxional anionic boron clusters B20(-/2-). *Chemistry - A European Journal*, **2012**, 18, 4510-2	4.8	76
637	Thermochemistry and electronic structure of small boron and boron oxide clusters and their anions. *Journal of Physical Chemistry A*, **2009**, 113, 4895-909	2.8	76
636	Decomposition mechanism of the polynitrogen N5 and N6 clusters and their ions. *Chemical Physics Letters*, **2001**, 335, 311-320	2.5	76
635	The boron buckyball has an unexpected Th symmetry. *Chemical Physics Letters*, **2008**, 450, 175-177	2.5	74
634	The Alcoholysis Reaction of Isocyanates Giving Urethanes: Evidence for a Multimolecular Mechanism. *Journal of Organic Chemistry*, **1998**, 63, 6878-6885	4.2	74
633	Theoretical study of formamide decomposition pathways. *Journal of Physical Chemistry A*, **2011**, 115, 841-51	2.8	72
632	Heats of formation of the Criegee formaldehyde oxide and dioxirane. *Chemical Physics Letters*, **2007**, 448, 183-188	2.5	70
631	The 2D-to-3D geometry hopping in small boron clusters: The charge effect. *Chemical Physics Letters* , **2013**, 577, 32-37	2.5	69
630	The S–H Bond Dissociation Enthalpies and Acidities of Para and Meta Substituted Thiophenols: A Quantum Chemical Study. *Journal of Physical Chemistry A*, **2003**, 107, 9182-9188	2.8	67
629	Nitromethane–Methyl Nitrite Rearrangement: A Persistent Discrepancy between Theory and Experiment. *Journal of Physical Chemistry A*, **2003**, 107, 4286-4291	2.8	67
628	In Search of Singlet Phosphinidenes. *Journal of Organic Chemistry*, **1996**, 61, 7077-7084	4.2	67
627	Influence of building block aromaticity in the determination of electronic properties of five-membered heterocyclic oligomers. *Physical Chemistry Chemical Physics*, **2002**, 4, 1522-1530	3.6	65

626	Theoretical study of the structure-property relationship in phosphole monomers. *Journal of Organic Chemistry*, **2000**, 65, 2631-6	4.2	65
625	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
624	High magnetic moments in manganese-doped silicon clusters. *Chemistry - A European Journal*, **2012**, 18, 15788-93	4.8	60
623	Disparate effects of Cu and V on structures of exohedral transition metal-doped silicon clusters: a combined far-infrared spectroscopic and computational study. *Journal of the American Chemical Society*, **2010**, 132, 15589-602	16.4	60
622	Experimental and Theoretical Evidence for a Concerted Catalysis by Water Clusters in the Hydrolysis of Isocyanates. *Journal of Organic Chemistry*, **1998**, 63, 6867-6877	4.2	59
621	Another Look at the Decomposition of Methyl Azide and Methanimine: How Is HCN Formed?. *The Journal of Physical Chemistry*, **1996**, 100, 6499-6503		58
620	Chromium-doped germanium clusters CrGen (n = 1-5): geometry, electronic structure, and topology of chemical bonding. *Journal of Physical Chemistry A*, **2007**, 111, 13544-53	2.8	58
619	Heats of formation of boron hydride anions and dianions and their ammonium salts [BnHmy-][NH4+]y with y=1-2. *Inorganic Chemistry*, **2007**, 46, 7561-70	5.1	56
618	Azidopentazole is Probably the Lowest-Energy N8 Species A Theoretical Study. *Chemische Berichte*, **1996**, 129, 1157-1159		56
617	Experimental Investigation of the Reaction between Nitric Oxide and Ketenyl Radicals (HCCO + NO): Rate Coefficient at T = 290-670 K and Product Distribution at 700 K. *The Journal of Physical Chemistry*, **1994**, 98, 8036-8043		56
616	Theoretical Characterization of the Reaction between Nitric Oxide and Ketenyl Radicals (HCCO + NO): CO versus CO2 Loss. *The Journal of Physical Chemistry*, **1994**, 98, 8030-8035		56
615	On the Asynchronism of Isocyanide Addition to Dipolarophiles: Application of Local Softness. *Journal of Organic Chemistry*, **1997**, 62, 6417-6419	4.2	54
614	A disk-aromatic bowl cluster B30: toward formation of boron buckyballs. *Chemical Communications*, **2014**, 50, 1558-60	5.8	53
613	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
612	Hydrogen Bonding between Phenol and Acetonitrile. *Journal of Physical Chemistry A*, **2002**, 106, 4267-427	2.8	52
611	The Boron conundrum: the case of cationic clusters B + n with n = 2 0. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	51
610	Difficulties of Density Functional Theory in Investigating Addition Reactions of the Hydrogen Atom. *The Journal of Physical Chemistry*, **1996**, 100, 18422-18425		51
609	Approach to regiochemistry using local softness in 1,3-dipolar cycloadditions. *Journal of Computational Chemistry*, **1998**, 19, 195-202	3.5	51

608	Chemical bonding in the boron buckyball. *Chemical Physics Letters*, **2008**, 461, 226-228	2.5	50
607	Nitrous oxide as a 1,3-dipole: a theoretical study of its cycloaddition mechanism. *Journal of Organic Chemistry*, **2001**, 66, 6096-103	4.2	50
606	Tuning the geometric structure by doping silicon clusters. *ChemPhysChem*, **2008**, 9, 703-6	3.2	49
605	Singlet□Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. *Journal of Physical Chemistry A*, **2004**, 108, 6554-6561	2.8	49
604	A density functional study of weakly bound hydrogen bonded complexes. *Chemical Physics*, **1998**, 232, 299-306	2.3	48
603	Structure□Property Relationships in Phosphole-Containing □Conjugated Systems: A Quantum Chemical Study. *Journal of Physical Chemistry A*, **2003**, 107, 838-846	2.8	48
602	Ionized Phenol and Its Isomers in the Gas Phase. *Journal of Physical Chemistry A*, **2001**, 105, 11582-11592	2.8	48
601	An ab initio study of the electronic spectrum of dichlorocarbene CCl2. *Chemical Physics Letters*, **1985**, 117, 295-300	2.5	48
600	A Theoretical Study of the CH2N System: Reactions in both Lowest Lying Doublet and Quartet States. *Journal of Physical Chemistry A*, **1998**, 102, 8013-8020	2.8	47
599	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
598	A particle on a hollow cylinder: the triple ring tubular cluster B27(+). *Physical Chemistry Chemical Physics*, **2014**, 16, 19470-8	3.6	45
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596	The triplet state of cytosine and its derivatives: electron impact and quantum chemical study. *Journal of Chemical Physics*, **2004**, 121, 11668-74	3.9	45
595	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
594	Distonic Isomers and Tautomers of the Adenine Cation Radical in the Gas Phase and Aqueous Solution. *Journal of Physical Chemistry A*, **2004**, 108, 9283-9293	2.8	44
593	Theoretical study of the vinyl azide-.upsilon.-triazole isomerization. *Journal of the American Chemical Society*, **1978**, 100, 3668-3674	16.4	43
592	□Conjugated Molecules Containing Naphtho[2,3-b]thiophene and Their Derivatives: Theoretical Design for Organic Semiconductors. *Journal of Physical Chemistry C*, **2013**, 117, 10175-10184	3.8	42
591	The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B112. *Physical Chemistry Chemical Physics*, **2011**, 13, 7524-33	3.6	41

590	The effect of the NH2 substituent on NH3: hydrazine as an alternative for ammonia in hydrogen release in the presence of boranes and alanes. *Physical Chemistry Chemical Physics*, **2009**, 11, 6339-44	3.6	41
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588	Theoretical study of the pentanitrogen cation (N5+). *Chemical Physics Letters*, **2000**, 317, 135-141	2.5	41
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586	From formamide to purine: a self-catalyzed reaction pathway provides a feasible mechanism for the entire process. *Journal of Physical Chemistry B*, **2013**, 117, 9333-42	3.4	40
585	The aromatic 8-electron cubic silicon clusters Be@Si(8), B@Si(8)(+), and C@Si(8)(2+). *Journal of Physical Chemistry A*, **2010**, 114, 7609-15	2.8	40
584	A concerted mechanism of proton transfer in green fluorescent protein. A theoretical study. *Chemical Physics Letters*, **2005**, 404, 250-256	2.5	40
583	Experimental and theoretical study of the reaction of the ethynyl radical with acetylene (HC?C+HC?CH). *Chemical Physics*, **2000**, 262, 243-252	2.3	40
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578	Theoretical study of the decomposition of formamide in the presence of water molecules. *Journal of Physical Chemistry A*, **2013**, 117, 2543-55	2.8	38
577	Efficient Calculation of Isotropic Hyperfine Constants of Phosphorus Radicals Using Density Functional Theory. *Journal of Physical Chemistry A*, **1997**, 101, 3174-3181	2.8	38
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575	The C-H and alpha(C-X) bond dissociation enthalpies of toluene, C6H5-CH2X (X = F, Cl), and their substituted derivatives: a DFT study. *Journal of Physical Chemistry A*, **2005**, 109, 10342-7	2.8	38
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561	Experimental observation and computational identification of Sc@Cu16+, a stable dopant-encapsulated copper cage. *Physical Review A*, **2007**, 76,	2.6	36
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