

# Zoltan Varga

## List of Publications by Year in descending order

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68  
papers

1,654  
citations

361045

20  
h-index

301761

39  
g-index

72  
all docs

72  
docs citations

72  
times ranked

1252  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | An improved potential energy surface and multi-temperature quasiclassical trajectory calculations of N <sub>2</sub> + N <sub>2</sub> dissociation reactions. <i>Journal of Chemical Physics</i> , 2015, 143, 054304.   | 1.2 | 178       |
| 2  | Global <i>ab initio</i> ground-state potential energy surface of N <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2013, 139, 044309.  | 1.2 | 175       |
| 3  | Halogen acceptors in hydrogen bonding. <i>Coordination Chemistry Reviews</i> , 2006, 250, 710-727.   | 9.5 | 171       |
| 4  | Assessment of electronic structure methods for the determination of the ground spin states of Fe(II), Fe(III) and Fe(IV) complexes. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 13049-13069.  | 1.3 | 100       |
| 5  | Potential energy surfaces for O + O <sub>2</sub> collisions. <i>Journal of Chemical Physics</i> , 2017, 147, 154312.   | 1.2 | 73        |
| 6  | Potential energy surfaces of quintet and singlet O <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2017, 147, 034301.  | 1.2 | 65        |
| 7  | Potential energy surface of triplet N <sub>2</sub> O <sub>2</sub> . <i>Journal of Chemical Physics</i> , 2016, 144, 024310.  | 1.2 | 63        |
| 8  | Potential energy surface of triplet O <sub>4</sub> . <i>Journal of Chemical Physics</i> , 2018, 148, 124314.   | 1.2 | 53        |
| 9  | Vibrational Energy Transfer and Collision-Induced Dissociation in O+O <sub>2</sub> Collisions. <i>Journal of Thermophysics and Heat Transfer</i> , 2019, 33, 797-807.  | 0.9 | 49        |
| 10 | Global triplet potential energy surfaces for the N <sub>2</sub> (X <sup>1</sup> Σ <sup>+</sup> ) + O(3P) → NO(X <sup>2</sup> Π) + N(4S) reaction. <i>Journal of Chemical Physics</i> , 2016, 144, 024309.  | 1.2 | 41        |
| 11 | Many-Body Permutationally Invariant Polynomial Neural Network Potential Energy Surface for N <sub>4</sub> . <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4822-4832.   | 2.3 | 40        |
| 12 | Diabatic States of Molecules. <i>Journal of Physical Chemistry A</i> , 2022, 126, 992-1018.  | 1.1 | 29        |
| 13 | Theoretical Study of the Structure and Bonding in ThC <sub>2</sub> and UC <sub>2</sub> . <i>Journal of Physical Chemistry A</i> , 2012, 116, 747-755.  | 1.1 | 28        |
| 14 | Multi-state pair-density functional theory. <i>Faraday Discussions</i> , 2020, 224, 348-372.   | 1.6 | 28        |
| 15 | Quasilinear Molecule par Excellence, SrCl <sub>2</sub> : Structure from High-Temperature Gas-Phase Electron Diffraction and Quantum-Chemical Calculations of Computed Structures of SrCl <sub>2</sub> ...Argon Complexes. <i>Chemistry - A European Journal</i> , 2006, 12, 8345-8357. | 1.7 | 27        |
| 16 | On the effect of 4f electrons on the structural characteristics of lanthanide trihalides: Computational and electron diffraction study of dysprosium trichloride. <i>Journal of Chemical Physics</i> , 2008, 128, 074301.  | 1.2 | 24        |
| 17 | Long-Range Effects in Oligopeptides. A Theoretical Study of the β <sup>2</sup> -Sheet Structure of Gln (n = 2~10). <i>Journal of Physical Chemistry A</i> , 2004, 108, 6869-6873.  | 1.1 | 23        |
| 18 | A quasiclassical trajectory study of the N <sub>2</sub> (X <sup>1</sup> Σ <sup>+</sup> ) + O(3P) → NO(X <sup>2</sup> Π) + N(4S) reaction. <i>Journal of Chemical Physics</i> , 2016, 144, 234314.  | 1.2 | 23        |

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|----|---|-----|-----------|
| 19 | Potential energy surfaces for high-energy N + O <sub>2</sub> collisions. Journal of Chemical Physics, 2021, 154, 084304.  | 1.2 | 23        |
| 20 | Prompt D <sup>0</sup> , D <sup>+</sup> , and D <sup>*+</sup> production in Pb–Pb collisions at $\sqrt{s_{\mathrm{NN}}}$ = 5.02 TeV. Journal of High Energy Physics, 2022, 2022, 1.                                      | 1.6 | 23        |
| 21 | The Elusive Structure of CrCl <sub>2</sub> —A Combined Computational and Gas-Phase Electron-Diffraction Study. Chemistry - A European Journal, 2008, 14, 5130-5143.   | 1.7 | 20        |
| 22 | Conservation of Angular Momentum in Direct Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 1135-1140.   | 2.1 | 20        |
| 23 | Permutationally Restrained Diabatization by Machine Intelligence. Journal of Chemical Theory and Computation, 2021, 17, 1106-1116.  | 2.3 | 20        |
| 24 | Structure and Other Molecular Properties of Actinide Trichlorides AnCl <sub>3</sub> (An = Th–Cm). Journal of Physical Chemistry A, 2013, 117, 11357-11363.  | 1.1 | 17        |
| 25 | Does the 4f Electron Configuration Affect Molecular Geometries? A Joint Computational, Vibrational Spectroscopic, and Electron Diffraction Study of Dysprosium Tribromide. Inorganic Chemistry, 2009, 48, 4143-4153.    | 1.9 | 16        |
| 26 | Substituent effects on long-range interactions in the $\beta$ -sheet structure of oligopeptides. Computational and Theoretical Chemistry, 2005, 755, 247-251.   | 1.5 | 15        |
| 27 | Gas-Phase Structures of Iron Trihalides: A Computational Study of all Iron Trihalides and an Electron Diffraction Study of Iron Trichloride. Inorganic Chemistry, 2010, 49, 1039-1045.                                  | 1.9 | 15        |
| 28 | Molecular Constants of Aluminum Monohalides: Caveats for Computations of Simple Inorganic Molecules. Journal of Physical Chemistry A, 2007, 111, 6-8.   | 1.1 | 13        |
| 29 | Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. Angewandte Chemie - International Edition, 2020, 59, 10826-10830.  | 7.2 | 13        |
| 30 | Comprehensive study of the structure of aluminum trihalides from electron diffraction and computation. Structural Chemistry, 2012, 23, 879-893.   | 1.0 | 12        |
| 31 | Hyper Open-Shell Excited Spin States of Transition-Metal Compounds: FeF <sub>2</sub> , FeF <sub>2</sub> –Ethane, and FeF <sub>2</sub> –Ethylene. Journal of Physical Chemistry A, 2018, 122, 2563-2579.                 | 1.1 | 12        |
| 32 | Direct diabatization based on nonadiabatic couplings: the N/D method. Physical Chemistry Chemical Physics, 2018, 20, 26643-26659.   | 1.3 | 12        |
| 33 | Production of pions, kaons, (anti-)protons and $\phi$ mesons in Xe–Xe collisions at $\sqrt{s_{\mathrm{NN}}}$ = 5.44 TeV. European Physical Journal C, 2021, 81, 1.  | 1.4 | 12        |
| 34 | Potential energy surface for high-energy N + N <sub>2</sub> collisions. Physical Chemistry Chemical Physics, 2021, 23, 26273-26284.   | 1.3 | 12        |
| 35 | Hydrogen bonding in peptide secondary structures. International Journal of Quantum Chemistry, 2005, 105, 302-312.   | 1.0 | 11        |
| 36 | Oviposition preferences of <i>Maculinea alcon</i> as influenced by aphid ( <i>Aphis gentianae</i> ) and fungal ( <i>Puccinia gentianae</i> ) infestation of larval host plants. Ecological Entomology, 2009, 34, 90-97. | 1.1 | 11        |

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|----|---|-----|-----------|
| 37 | Hyper Open-Shell States: The Lowest Excited Spin States of O Atom, Fe <sup>2+</sup> Ion, and FeF <sub>2</sub> . Journal of the American Chemical Society, 2017, 139, 12569-12578.   | 6.6 | 11        |
| 38 | On the thermal expansion of molecules. Structural Chemistry, 2011, 22, 111-121.   | 1.0 | 10        |
| 39 | Quasiclassical Trajectory Analysis of the N <sub>2</sub> + N <sub>2</sub> Reaction Using a New Ab Initio Potential Energy Surface., 2014, , .   |     | 10        |
| 40 | Modification of Jet Structure in High-Multiplicity pp Collisions due to Multiple-Parton Interactions and Observing a Multiplicity-Independent Characteristic Jet Size. Advances in High Energy Physics, 2019, 2019, 1-12. | 0.5 | 10        |
| 41 | Water Catalysis of the Reaction of Methanol with OH Radical in the Atmosphere is Negligible. Angewandte Chemie, 2020, 132, 10918-10922.   | 1.6 | 10        |
| 42 | Molecular Geometry of Vanadium Dichloride and Vanadium Trichloride: A Gas-Phase Electron Diffraction and Computational Study. Inorganic Chemistry, 2010, 49, 2816-2821.   | 1.9 | 9         |
| 43 | Iron dihalides: structures and thermodynamic properties from computation and an electron diffraction study of iron diiodide. Structural Chemistry, 2011, 22, 327-336.   | 1.0 | 9         |
| 44 | Is the Inversion of Phosphorus Trihalides (PF <sub>3</sub> , PCl <sub>3</sub> , PBr <sub>3</sub> , and PI <sub>3</sub> ) a Diradical Process?. Journal of Physical Chemistry A, 2019, 123, 301-312.                       | 1.1 | 9         |
| 45 | Group 14 structural variations: perhalo derivatives of the "metallenes", dicarbenes, disilenes, digermenes, distannenes, and diplumbenes. Structural Chemistry, 2013, 24, 837-850.  | 1.0 | 8         |
| 46 | The NaDyBr <sub>4</sub> complex; its molecular structure and thermodynamic properties. Structural Chemistry, 2006, 17, 225-233.   | 1.0 | 7         |
| 47 | Vapor phase tin diiodide: its structure and thermodynamics, a computational study. Structural Chemistry, 2007, 18, 641-648.   | 1.0 | 7         |
| 48 | Curious matrix effects: a computational, electron diffraction, and vibrational spectroscopic study of dysprosium triiodide. Dalton Transactions, 2010, 39, 6221.  | 1.6 | 7         |
| 49 | Structures and thermodynamic properties of aluminum oxyhalides: a computational study. Structural Chemistry, 2008, 19, 595-602.   | 1.0 | 6         |
| 50 | About the structure of CH <sub>5</sub> <sup>+</sup> and structural variations in related systems. Structural Chemistry, 2017, 28, 297-301.  | 1.0 | 6         |
| 51 | On the thermal expansion of molecules: a sequel. Structural Chemistry, 2011, 22, 1065-1066.   | 1.0 | 5         |
| 52 | Molecular Structure and Vibrational Spectra of Mixed MDyX <sub>4</sub> (M = Li, Na, K, Rb, Cs; X = F,) Tj ETQq0 0 0 rgBT /Overlock 10<br>Inorganic Chemistry, 2012, 51, 543-556.  | 1.9 | 5         |
| 53 | Chemistry, commentary and community: Discussion of "The NaDyBr <sub>4</sub> complex: its molecular structure and thermodynamic properties" by Varga and Hargittai. Structural Chemistry, 2007, 18, 269-271.               | 1.0 | 4         |
| 54 | Jet Structure Studies in Small Systems. Universe, 2019, 5, 132.   | 0.9 | 4         |

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|----|--|-----|-----------|
| 55 | Metal–ligand interactions in complexes of cyclen-based ligands with Bi and Ac. Structural Chemistry, 2021, 32, 1719-1731.  | 1.0 | 3         |
| 56 | Thiolated cationic poly(aspartamides) with side group dependent gelation properties for the delivery of anionic polyelectrolytes. Journal of Materials Chemistry B, 2022, 10, 5946-5957. | 2.9 | 3         |
| 57 | Paradigms and paradoxes: the conformation of the fundamental unit of hyaluronic acid. Structural Chemistry, 2010, 21, 1211-1214.   | 1.0 | 2         |
| 58 | Singlet–triplet competition in the low-lying energy states of C <sub>4</sub> O <sub>4</sub> <sup>n</sup> S <sub>n</sub> (n=1–3) molecules. Structural Chemistry, 2015, 26, 1229-1240.    | 1.0 | 2         |
| 59 | B <sub>2</sub> N <sub>2</sub> O <sub>4</sub> : Prediction of a Magnetic Ground State for a Light Main-Group Molecule. Inorganic Chemistry, 2015, 54, 8552-8559.                          | 1.9 | 2         |
| 60 | Significant $\pi$ -stacking effect between 2,4,6-triphenyl-1-phosphabenzene. Structural Chemistry, 2017, 28, 1243-1253.  | 1.0 | 2         |
| 61 | Multiplicity Dependence of the Jet Structures in pp Collisions at LHC Energies. Proceedings (mdpi), 2019, 10, 3.   | 0.2 | 2         |
| 62 | H <sub>2</sub> O coordination in macropa complexes of f elements (Ac, La, Lu): feasibility of the 11th coordination site. Structural Chemistry, 2021, 32, 643-653.                       | 1.0 | 2         |
| 63 | Investigation of self-excited ultrahigh speed induction generators for Distributed Generation Systems. , 2011, , .   |     | 1         |
| 64 | The role of the underlying event in the $\hat{\chi}_c^+$ enhancement in high-energy pp collisions. Journal of Physics G: Nuclear and Particle Physics, 2022, 49, 075005.                 | 1.4 | 1         |
| 65 | Time average approach for the calculation of quasi-subharmonics of PWM technique in ultra high speed AC motor supply. , 2010, , .  |     | 0         |
| 66 | Development of animated material for e-learning in solar powered electric vehicles. , 2013, , .  |     | 0         |
| 67 | Wind energy penetration into distributed generation and its static and dynamic features. , 2014, , .   |     | 0         |
| 68 | The Partonic Origin of Multiplicity Scaling in Heavy and Light Flavor Jets. Symmetry, 2022, 14, 1379.  | 1.1 | 0         |