

Vitaly A Rassolov

List of Publications by Year in descending order

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87
papers

15,958
citations

159358

30
h-index

49773

87
g-index

91
all docs

91
docs citations

91
times ranked

13803
citing authors

#	ARTICLE	IF	CITATIONS
1	Gaussian-3 (G3) theory for molecules containing first and second-row atoms. <i>Journal of Chemical Physics</i> , 1998, 109, 7764-7776.	1.2	2,746
2	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 3172-3191.	1.3	2,597
3	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
4	6-31G* basis set for third-row atoms. <i>Journal of Computational Chemistry</i> , 2001, 22, 976-984.	1.5	1,891
5	6-31G* basis set for atoms K through Zn. <i>Journal of Chemical Physics</i> , 1998, 109, 1223-1229.	1.2	1,766
6	Gaussian-3 theory using reduced Møller-Plesset order. <i>Journal of Chemical Physics</i> , 1999, 110, 4703-4709.	1.2	1,201
7	Q-Chem 2.0: a high-performance ab initio electronic structure program package. <i>Journal of Computational Chemistry</i> , 2000, 21, 1532-1548.	1.5	617
8	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
9	Extension of Gaussian-3 theory to molecules containing third-row atoms K, Ca, Ga–Kr. <i>Journal of Chemical Physics</i> , 2001, 114, 9287-9295.	1.2	152
10	Supramolecular Structural Variations with Changes in Anion and Solvent in Silver(I) Complexes of a Semirigid, Bitopic Tris(pyrazolyl)methane Ligand. <i>Inorganic Chemistry</i> , 2004, 43, 537-554.	1.9	125
11	A geminal model chemistry. <i>Journal of Chemical Physics</i> , 2002, 117, 5978-5987.	1.2	120
12	Highly Organized Structures and Unusual Magnetic Properties of Paddlewheel Copper(II) Carboxylate Dimers Containing the π - π Stacking, 1,8-Naphthalimide Synthon. <i>Inorganic Chemistry</i> , 2009, 48, 8911-8924.	1.9	94
13	Energy conserving approximations to the quantum potential: Dynamics with linearized quantum force. <i>Journal of Chemical Physics</i> , 2004, 120, 1181-1190.	1.2	77
14	Absorption Spectrum, Mass Spectrometric Properties, and Electronic Structure of 1,2-Benzoquinone. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7470-7478.	1.1	69
15	Geminal model chemistry II. Perturbative corrections. <i>Journal of Chemical Physics</i> , 2004, 120, 10385-10394.	1.2	65
16	Semiclassical dynamics based on quantum trajectories. <i>Chemical Physics Letters</i> , 2002, 364, 562-567.	1.2	59
17	Geminal model chemistry. IV. Variational and size consistent pure spin states. <i>Journal of Chemical Physics</i> , 2007, 127, 044104.	1.2	57
18	Quantum dynamics with Bohmian trajectories: energy conserving approximation to the quantum potential. <i>Chemical Physics Letters</i> , 2003, 376, 358-363.	1.2	56

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19	6s ² 6p ⁴ basis set for third-row atoms. <i>Journal of Computational Chemistry</i> , 2001, 22, 976-984.	1.5	56
20	Behavior of electronic wave functions near cusps. <i>Journal of Chemical Physics</i> , 1996, 104, 9908-9912.	1.2	50
21	The Stable Pentamethylcyclopentadienyl Cation. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1429-1431.	7.2	49
22	Semiclassical dynamics with quantum trajectories: Formulation and comparison with the semiclassical initial value representation propagator. <i>Journal of Chemical Physics</i> , 2003, 118, 2482.	1.2	49
23	Bohmian dynamics on subspaces using linearized quantum force. <i>Journal of Chemical Physics</i> , 2004, 120, 6815-6825.	1.2	45
24	Semiclassical nonadiabatic dynamics with quantum trajectories. <i>Physical Review A</i> , 2005, 71, .	1.0	43
25	The relativistic Dirac-Coulomb-Fock effect on atomization energies. <i>Journal of Chemical Physics</i> , 1999, 110, 7123-7126.	1.2	39
26	1,8-Naphthalimide Synthon in Silver Coordination Chemistry: Control of Supramolecular Arrangement. <i>Crystal Growth and Design</i> , 2006, 6, 2758-2768.	1.4	39
27	Geminal model chemistry III: Partial spin restriction. <i>Journal of Chemical Physics</i> , 2007, 126, 234112.	1.2	38
28	Quantum Trajectory Dynamics in Arbitrary Coordinates. <i>Journal of Physical Chemistry A</i> , 2006, 110, 5530-5536.	1.1	33
29	Crystal Growth of Two New Niobates, La ₂ KNbO ₆ and Nd ₂ KNbO ₆ : Structural, Dielectric, Photophysical, and Photocatalytic Properties. <i>Chemistry of Materials</i> , 2008, 20, 3327-3335.	3.2	32
30	Binuclear Aromatic C-H Bond Activation at a Dirhenium Site. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 1324-1327.	7.2	31
31	Electron correlation in chemical bonds. <i>Journal of Chemical Physics</i> , 2000, 112, 4014-4019.	1.2	29
32	Modified quantum trajectory dynamics using a mixed wave function representation. <i>Journal of Chemical Physics</i> , 2004, 121, 8711-8715.	1.2	29
33	Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(P3,D1)+H ₂ system. <i>Journal of Chemical Physics</i> , 2006, 124, 244307.	1.2	29
34	Computational complexity in quantum chemistry. <i>Chemical Physics Letters</i> , 2008, 464, 262-264.	1.2	29
35	New operators for electronic density calculation. I. Derivations and formal analysis. <i>Journal of Chemical Physics</i> , 1996, 105, 1470-1478.	1.2	27
36	Facile C-H Bond Formation by Reductive Elimination at a Dinuclear Metal Site. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 11006-11009.	7.2	27

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37	Monte Carlo Simulation of Electron Thermalization Distribution in Liquid Hydrocarbons: Effects of Inverse Collisions and of an External Electric Field. <i>Journal of Physical Chemistry B</i> , 2001, 105, 1430-1437.	1.2	25
38	An ab initio linear electron correlation functional. <i>Journal of Chemical Physics</i> , 1999, 110, 3672-3677.	1.2	23
39	Semiclassical nonadiabatic dynamics using a mixed wave-function representation. <i>Journal of Chemical Physics</i> , 2005, 123, 174108.	1.2	23
40	Stable long-time semiclassical description of zero-point energy in high-dimensional molecular systems. <i>Journal of Chemical Physics</i> , 2008, 129, 024109.	1.2	23
41	Local spin from strongly orthogonal geminal wavefunctions. <i>Molecular Physics</i> , 2015, 113, 249-259.	0.8	23
42	The electronic mean field configuration interaction method: III – the $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si46.gif" display="inline" overflow="scroll" \rangle \langle \text{mml:mrow} \langle \text{mml:mi} \rangle \text{p} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle$ -orthogonality constraint. <i>Chemical Physics Letters</i> , 2010, 487, 147-152.	1.2	21
43	New operators for electronic density calculation. II. Application to hydrogen, first-row atoms, and first-row diatomic hydrides. <i>Journal of Chemical Physics</i> , 1996, 105, 1479-1491.	1.2	20
44	Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Sc–Zn. <i>Journal of Chemical Physics</i> , 2008, 128, 144122.	1.2	20
45	Estimation of the Ground State Energy of an Atomic Solid by Employing Quantum Trajectory Dynamics with Friction. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2891-2899.	2.3	19
46	Unsaturated Triosmium Carbonyl Cluster Complexes with Bridging Aryl Ligands: Structures, Bonding, and Transformations. <i>Organometallics</i> , 2013, 32, 6368-6378.	1.1	18
47	Semiclassical nonadiabatic dynamics of NaFH with quantum trajectories. <i>Chemical Physics Letters</i> , 2007, 446, 395-400.	1.2	15
48	Tetraruthenium carbonyl complexes containing germyl and stannyl ligands from the reactions of Ru ₄ (CO) ₁₃ (1/4-H) ₂ with HGePh ₃ and HSnPh ₃ . <i>Journal of Organometallic Chemistry</i> , 2013, 730, 20-31.	0.8	14
49	Oxygen Anion Solubility as a Factor in Molten Flux Crystal Growth, Synthesis, and Characterization of Four New Reduced Lanthanide Molybdenum Oxides: Ce _{4.918(3)} Mo ₃ O ₁₆ , Pr _{4.880(3)} Mo ₃ O ₁₆ , Nd _{4.910(3)} Mo ₃ O ₁₆ , and Sm _{4.952(3)} Mo ₃ O ₁₆ . <i>Crystal Growth and Design</i> , 2016, 16, 4225-4231.	1.4	13
50	Spin density in first-row atoms from the Hiller-Sucher-Feinberg identity. <i>Theoretica Chimica Acta</i> , 1995, 91, 1-15.	0.9	11
51	The definition of core electrons. <i>Chemical Physics Letters</i> , 2001, 350, 573-576.	1.2	11
52	Synthesis and Transformations of Triosmium Carbonyl Cluster Complexes Containing Bridging Aryl Ligands. <i>Organometallics</i> , 2012, 31, 2961-2964.	1.1	11
53	SS <i>p</i> C: A strongly orthogonal geminal method with relaxed strong orthogonality. <i>Journal of Chemical Physics</i> , 2014, 141, 164112.	1.2	11
54	Spin density in first-row diatomic hydrides from the Hiller–Sucher–Feinberg identity. <i>Journal of Chemical Physics</i> , 1995, 103, 10058-10069.	1.2	10

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55	New operators for calculation of indirect nuclear spin-spin coupling constants. <i>Journal of Chemical Physics</i> , 1997, 107, 5488-5495.	1.2	10
56	Semiempirical models for image electrostatics. I. Bare external charge. <i>Journal of Chemical Physics</i> , 2001, 114, 2062-2066.	1.2	10
57	Stabilization of Quantum Energy Flows within the Approximate Quantum Trajectory Approach. <i>Journal of Physical Chemistry A</i> , 2007, 111, 10251-10255.	1.1	10
58	Dynamic Rotation of Bridging Aryl Ligands in Unsaturated Metal Carbonyl Cluster Complexes. <i>Organometallics</i> , 2013, 32, 1587-1590.	1.1	10
59	Fluorescence Polarization Measurements to Probe Alignment of a Bithiophene Dye in One-Dimensional Channels of Self-Assembled Phenylethynylene Bis-Urea Macrocyclic Crystals. <i>Journal of Physical Chemistry C</i> , 2017, 121, 18102-18109.	1.5	10
60	Large transition state stabilization from a weak hydrogen bond. <i>Chemical Science</i> , 2020, 11, 7487-7494.	3.7	10
61	Lithium atom spin density from the Hiller-Sucher-Feinberg identity. <i>Theoretica Chimica Acta</i> , 1994, 88, 339-349.	0.9	9
62	Dynamics in the quantum/classical limit based on selective use of the quantum potential. <i>Journal of Chemical Physics</i> , 2014, 141, 234107.	1.2	9
63	Synthesis and Reactivity of Electronically Unsaturated Dirhenium Carbonyl Compounds Containing Bridging Gold-Carbene Groups. <i>Inorganic Chemistry</i> , 2016, 55, 10475-10483.	1.9	9
64	The diagonal Born-Oppenheimer correction to molecular dynamical properties. <i>Chemical Physics Letters</i> , 2001, 333, 459-464.	1.2	8
65	Fermi Contact Spin Density Calculations of Aromatic Radicals. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20648-20658.	1.5	8
66	Density functional model of multireference systems based on geminals. <i>Chemical Physics Letters</i> , 2012, 543, 205-207.	1.2	8
67	Approximate quantum trajectory dynamics for reactive processes in condensed phase. <i>Molecular Simulation</i> , 2015, 41, 86-106.	0.9	7
68	Binuclear Aromatic C-H Bond Activation at a Dirhenium Site. <i>Angewandte Chemie</i> , 2016, 128, 1346-1349.	1.6	6
69	Quantum Trajectory Dynamics Based on Local Approximations to the Quantum Potential and Force. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3906-3916.	2.3	6
70	Description of electronic excited states using electron correlation operator. <i>Journal of Chemical Physics</i> , 2013, 139, 104111.	1.2	5
71	Correlation between the Stability of Substituted Cobaltocenium and Molecular Descriptors. <i>Journal of Physical Chemistry A</i> , 2022, 126, 80-87.	1.1	5
72	Analytical potential energy surface for O+C ₂ H ₂ system. <i>Chemical Physics Letters</i> , 2013, 588, 22-26.	1.2	4

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73	The Stable Pentamethylcyclopentadienyl Cation. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 1642-1642.	7.2	3
74	Symmetrization of the nuclear wavefunctions defined by the quantum trajectory dynamics. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	0.5	3
75	Multicenter transformations of the methyl ligand in CH ₃ Os ₃ Au carbonyl cluster complexes: Synthesis, characterization and DFT analyses. <i>Journal of Organometallic Chemistry</i> , 2016, 812, 95-107.	0.8	3
76	Stability Analysis of Substituted Cobaltocenium [Bis(cyclopentadienyl)cobalt(III)] Employing Chemistry-Informed Neural Networks. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3099-3110.	2.3	3
77	Experimental and Theoretical Examination of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3493-3504.	1.2	3
78	Description of metals based on localized electrons. <i>Chemical Physics Letters</i> , 2002, 363, 219-225.	1.2	2
79	Applicability criterion for semiclassical Bohmian dynamics. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1057-1064.	1.0	2
80	Semiclassical electron correlation operator. <i>Journal of Chemical Physics</i> , 2009, 131, 204102.	1.2	2
81	OH Radical as a Probe of the Spin Polarizability in 1- and 2-Naphthol. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4015-4022.	1.1	2
82	Molecular dynamics with nuclear quantum effects: Approximations to the quantum force. <i>Annual Reports in Computational Chemistry</i> , 2020, , 41-90.	0.9	2
83	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
84	Alternative Fermi Contact Operators for EPR and NMR. , 2004, , 493-504.		1
85	Harmonic electron correlation operator. <i>Journal of Chemical Physics</i> , 2011, 135, 034111.	1.2	1
86	Local Measure of Quantum Effects in Quantum Dynamics. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4653-4667.	1.1	1
87	Modeling the Ligand Effect on the Structure of CYP 450 Within the Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2818-2824.	1.1	1