Vitaly A Rassolov

List of Publications by Year
in descending order

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87 papers	15,958 citations	159585 30 h-index	49909 87 g-index
91 all docs	91 docs citations	91 times ranked	13803 citing authors

#	Article	IF	Citations
1	Correlation between the Stability of Substituted Cobaltocenium and Molecular Descriptors. Journal of Physical Chemistry A, 2022, 126, 80-87.	2.5	5
2	Stability Analysis of Substituted Cobaltocenium [Bis(cyclopentadienyl)cobalt(III)] Employing Chemistry-Informed Neural Networks. Journal of Chemical Theory and Computation, 2022, 18, 3099-3110.	5.3	3
3	Modeling the Ligand Effect on the Structure of CYP 450 Within the Density Functional Theory. Journal of Physical Chemistry A, 2022, 126, 2818-2824.	2.5	1
4	Experimental and Theoretical Examination of the Kinetic Isotope Effect in Cytochrome P450 Decarboxylase OleT. Journal of Physical Chemistry B, 2022, 126, 3493-3504.	2.6	3
5	Local Measure of Quantum Effects in Quantum Dynamics. Journal of Physical Chemistry A, 2021, 125, 4653-4667.	2.5	1
6	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
7	Molecular dynamics with nuclear quantum effects: Approximations to the quantum force. Annual Reports in Computational Chemistry, 2020, , 41-90.	1.7	2
8	Large transition state stabilization from a weak hydrogen bond. Chemical Science, 2020, 11, 7487-7494.	7.4	10
9	Quantum Trajectory Dynamics Based on Local Approximations to the Quantum Potential and Force. Journal of Chemical Theory and Computation, 2019, 15, 3906-3916.	5.3	6
10	OH Radical as a Probe of the Spin Polarizability in 1- and 2-Naphthol. Journal of Physical Chemistry A, 2018, 122, 4015-4022.	2.5	2
11	Fluorescence Polarization Measurements to Probe Alignment of a Bithiophene Dye in One-Dimensional Channels of Self-Assembled Phenylethynylene Bis-Urea Macrocycle Crystals. Journal of Physical Chemistry C, 2017, 121, 18102-18109.	3.1	10
12	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)}Mo₃O₁₆, Pr_{4.880(3)}Mo₃O₁₆, Nd_{4.910(3)}Mo₃O₁₆, and Sm_{4.952(3)}Mo₃O₁₆. Crystal Growth and Design, 2016, 16, 4225-4231.	3.0	13
13	Binuclear Aromatic Câ€'H Bond Activation at a Dirhenium Site. Angewandte Chemie, 2016, 128, 1346-1349.	2.0	6
14	Synthesis and Reactivity of Electronically Unsaturated Dirhenium Carbonyl Compounds Containing Bridging Gold-Carbene Groups. Inorganic Chemistry, 2016, 55, 10475-10483.	4.0	9
15	Symmetrization of the nuclear wavefunctions defined by the quantum trajectory dynamics. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	3
16	Binuclear Aromatic Câ€'H Bond Activation at a Dirhenium Site. Angewandte Chemie - International Edition, 2016, 55, 1324-1327.	13.8	31
17	Multicenter transformations of the methyl ligand in CH3Os3Au carbonyl cluster complexes: Synthesis, characterization and DFT analyses. Journal of Organometallic Chemistry, 2016, 812, 95-107.	1.8	3
18	Estimation of the Ground State Energy of an Atomic Solid by Employing Quantum Trajectory Dynamics with Friction. Journal of Chemical Theory and Computation, 2015, 11, 2891-2899.	5.3	19

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19	Approximate quantum trajectory dynamics for reactive processes in condensed phase. Molecular Simulation, 2015, 41, 86-106.	2.0	7
20	Local spin from strongly orthogonal geminal wavefunctions. Molecular Physics, 2015, 113, 249-259.	1.7	23
21	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
22	Dynamics in the quantum/classical limit based on selective use of the quantum potential. Journal of Chemical Physics, 2014, 141, 234107.	3.0	9
23	Facile Cï£¿H Bond Formation by Reductive Elimination at a Dinuclear Metal Site. Angewandte Chemie - International Edition, 2014, 53, 11006-11009.	13.8	27
24	SSpG: A strongly orthogonal geminal method with relaxed strong orthogonality. Journal of Chemical Physics, 2014, 141, 164112.	3.0	11
25	Analytical potential energy surface for O+C2H2 system. Chemical Physics Letters, 2013, 588, 22-26.	2.6	4
26	Tetraruthenium carbonyl complexes containing germyl and stannyl ligands from the reactions of Ru4(CO)13(Î¼-H)2 with HGePh3 and HSnPh3. Journal of Organometallic Chemistry, 2013, 730, 20-31.	1.8	14
27	Dynamic Rotation of Bridging Aryl Ligands in Unsaturated Metal Carbonyl Cluster Complexes. Organometallics, 2013, 32, 1587-1590.	2.3	10
28	Unsaturated Triosmium Carbonyl Cluster Complexes with Bridging Aryl Ligands: Structures, Bonding, and Transformations. Organometallics, 2013, 32, 6368-6378.	2.3	18
29	Description of electronic excited states using electron correlation operator. Journal of Chemical Physics, 2013, 139, 104111.	3.0	5
30	Synthesis and Transformations of Triosmium Carbonyl Cluster Complexes Containing Bridging Aryl Ligands. Organometallics, 2012, 31, 2961-2964.	2.3	11
31	Density functional model of multireference systems based on geminals. Chemical Physics Letters, 2012, 543, 205-207.	2.6	8
32	Harmonic electron correlation operator. Journal of Chemical Physics, 2011, 135, 034111.	3.0	1
33	The electronic mean field configuration interaction method: III â€“ the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si46.gif" display="inline" overflow="scroll"><mml:mrow><mml:mi>p</mml:mi></mml:mrow></mml:math>-orthogonality constraint. Chemical Physics Letters, 2010, 487, 147-152.	2.6	21
34	Fermi Contact Spin Density Calculations of Aromatic Radicals. Journal of Physical Chemistry C, 2010, 114, 20648-20658.	3.1	8
35	Absorption Spectrum, Mass Spectrometric Properties, and Electronic Structure of 1,2-Benzoquinone. Journal of Physical Chemistry A, 2010, 114, 7470-7478.	2.5	69
36	Semiclassical electron correlation operator. Journal of Chemical Physics, 2009, 131, 204102.	3.0	2

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37	Highly Organized Structures and Unusual Magnetic Properties of Paddlewheel Copper(II) Carboxylate Dimers Containing the Ï€âˆ'Ï€ Stacking, 1,8-Naphthalimide Synthon. Inorganic Chemistry, 2009, 48, 8911-8924.	4.0	94
38	Computational complexity in quantum chemistry. Chemical Physics Letters, 2008, 464, 262-264.	2.6	29
39	Crystal Growth of Two New Niobates, La2KNbO6 and Nd2KNbO6: Structural, Dielectric, Photophysical, and Photocatalytic Properties. Chemistry of Materials, 2008, 20, 3327-3335.	6.7	32
40	Stable long-time semiclassical description of zero-point energy in high-dimensional molecular systems. Journal of Chemical Physics, 2008, 129, 024109.	3.0	23
41	Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Scâ€"Zn. Journal of Chemical Physics, 2008, 128, 144122.	3.0	20
42	Geminal model chemistry. IV. Variational and size consistent pure spin states. Journal of Chemical Physics, 2007, 127, 044104.	3.0	57
43	Geminal model chemistry III: Partial spin restriction. Journal of Chemical Physics, 2007, 126, 234112.	3.0	38
44	Stabilization of Quantum Energy Flows within the Approximate Quantum Trajectory Approach. Journal of Physical Chemistry A, 2007, 111, 10251-10255.	2.5	10
45	Semiclassical nonadiabatic dynamics of NaFH with quantum trajectories. Chemical Physics Letters, 2007, 446, 395-400.	2.6	15
46	1,8-Naphthalimide Synthon in Silver Coordination Chemistry:â€‰ Control of Supramolecular Arrangement. Crystal Growth and Design, 2006, 6, 2758-2768.	3.0	39
47	Quantum Trajectory Dynamics in Arbitrary Coordinatesâ€. Journal of Physical Chemistry A, 2006, 110, 5530-5536.	2.5	33
48	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	2.8	2,597
49	Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(P3,D1)+H2 system. Journal of Chemical Physics, 2006, 124, 244307.	3.0	29
50	Semiclassical nonadiabatic dynamics with quantum trajectories. Physical Review A, 2005, 71, .	2.5	43
51	Semiclassical nonadiabatic dynamics using a mixed wave-function representation. Journal of Chemical Physics, 2005, 123, 174108.	3.0	23
52	Bohmian dynamics on subspaces using linearized quantum force. Journal of Chemical Physics, 2004, 120, 6815-6825.	3.0	45
53	Modified quantum trajectory dynamics using a mixed wave function representation. Journal of Chemical Physics, 2004, 121, 8711-8715.	3.0	29
54	Energy conserving approximations to the quantum potential: Dynamics with linearized quantum force. Journal of Chemical Physics, 2004, 120, 1181-1190.	3.0	77

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55	Applicability criterion for semiclassical Bohmian dynamics. International Journal of Quantum Chemistry, 2004, 100, 1057-1064.	2.0	2
56	Geminal model chemistry II. Perturbative corrections. Journal of Chemical Physics, 2004, 120, 10385-10394.	3.0	65
57	Alternative Fermi Contact Operators for EPR and NMR. , 2004, , 493-504.		1
58	Supramolecular Structural Variations with Changes in Anion and Solvent in Silver(I) Complexes of a Semirigid, Bitopic Tris(pyrazolyl)methane Ligand. Inorganic Chemistry, 2004, 43, 537-554.	4.0	125
59	Quantum dynamics with Bohmian trajectories: energy conserving approximation to the quantum potential. Chemical Physics Letters, 2003, 376, 358-363.	2.6	56
60	Semiclassical dynamics with quantum trajectories: Formulation and comparison with the semiclassical initial value representation propagator. Journal of Chemical Physics, 2003, 118, 2482.	3.0	49
61	A geminal model chemistry. Journal of Chemical Physics, 2002, 117, 5978-5987.	3.0	120
62	The Stable Pentamethylcyclopentadienyl Cation. Angewandte Chemie - International Edition, 2002, 41, 1429-1431.	13.8	49
63	The Stable Pentamethylcyclopentadienyl Cation. Angewandte Chemie - International Edition, 2002, 41, 1642-1642.	13.8	3
64	Description of metals based on localized electrons. Chemical Physics Letters, 2002, 363, 219-225.	2.6	2
65	Semiclassical dynamics based on quantum trajectories. Chemical Physics Letters, 2002, 364, 562-567.	2.6	59
66	Monte Carlo Simulation of Electron Thermalization Distribution in Liquid Hydrocarbons:â€‰ Effects of Inverse Collisions and of an External Electric Field. Journal of Physical Chemistry B, 2001, 105, 1430-1437.	2.6	25
67	6-31G* basis set for third-row atoms. Journal of Computational Chemistry, 2001, 22, 976-984.	3.3	1,891
68	The definition of core electrons. Chemical Physics Letters, 2001, 350, 573-576.	2.6	11
69	The diagonal Bornâ€“Oppenheimer correction to molecular dynamical properties. Chemical Physics Letters, 2001, 333, 459-464.	2.6	8
70	Extension of Gaussian-3 theory to molecules containing third-row atoms K, Ca, Gaâ€“Kr. Journal of Chemical Physics, 2001, 114, 9287-9295.	3.0	152
71	Semiempirical models for image electrostatics. I. Bare external charge. Journal of Chemical Physics, 2001, 114, 2062-2066.	3.0	10
72	6â€31G* basis set for thirdâ€row atoms. Journal of Computational Chemistry, 2001, 22, 976-984.	3.3	56

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73	Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548.	3.3	617
74	Electron correlation in chemical bonds. Journal of Chemical Physics, 2000, 112, 4014-4019.	3.0	29
75	Q-Chem 2.0: a high-performance ab initio electronic structure program package. , 2000, 21, 1532.		2
76	An ab initio linear electron correlation functional. Journal of Chemical Physics, 1999, 110, 3672-3677.	3.0	23
77	The relativistic Diracâ€“Coulombâ€“Fock effect on atomization energies. Journal of Chemical Physics, 1999, 110, 7123-7126.	3.0	39
78	Gaussian-3 theory using reduced Mo/ller-Plesset order. Journal of Chemical Physics, 1999, 110, 4703-4709.	3.0	1,201
79	Gaussian-3 (G3) theory for molecules containing first and second-row atoms. Journal of Chemical Physics, 1998, 109, 7764-7776.	3.0	2,746
80	6-31G* basis set for atoms K through Zn. Journal of Chemical Physics, 1998, 109, 1223-1229.	3.0	1,766
81	New operators for calculation of indirect nuclear spinâ€“spin coupling constants. Journal of Chemical Physics, 1997, 107, 5488-5495.	3.0	10
82	Behavior of electronic wave functions near cusps. Journal of Chemical Physics, 1996, 104, 9908-9912.	3.0	50
83	New operators for electronic density calculation. II. Application to hydrogen, firstâ€row atoms, and firstâ€row diatomic hydrides. Journal of Chemical Physics, 1996, 105, 1479-1491.	3.0	20
84	New operators for electronic density calculation. I. Derivations and formal analysis. Journal of Chemical Physics, 1996, 105, 1470-1478.	3.0	27
85	Spin density in firstâ€row diatomic hydrides from the Hillerâ€“Sucherâ€“Feinberg identity. Journal of Chemical Physics, 1995, 103, 10058-10069.	3.0	10
86	Spin density in first-row atoms from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1995, 91, 1-15.	0.8	11
87	Lithium atom spin density from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1994, 88, 339-349.	0.8	9