# Vitaly A Rassolov

List of Publications by Year
in descending order

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Version: 2024-02-01

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

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Gaussian-3 (G3) theory for molecules containing first and second-row atoms. Journal of Chemical Physics, 1998, 109, 7764-7776. | 3.0 | 2,746 |
| 2 | Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191. | 2.8 | 2,597 |
| 3 | Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215. | 1.7 | 2,561 |
| 4 | 6-31G* basis set for third-row atoms. Journal of Computational Chemistry, 2001, 22, 976-984. | 3.3 | 1,891 |
| 5 | 6-31G* basis set for atoms K through Zn. Journal of Chemical Physics, 1998, 109, 1223-1229. | 3.0 | 1,766 |
| 6 | Gaussian-3 theory using reduced Mo/ller-Plesset order. Journal of Chemical Physics, 1999, 110, 4703-4709. | 3.0 | 1,201 |
| 7 | Q-Chem 2.0: a high-performanceab initio electronic structure program package. Journal of Computational Chemistry, 2000, 21, 1532-1548. | 3.3 | 617 |
| 8 | 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 |
| 9 | 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 |
| 10 | 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 |
| 11 | A geminal model chemistry. Journal of Chemical Physics, 2002, 117, 5978-5987. | 3.0 | 120 |
| 12 | Highly Organized Structures and Unusual Magnetic Properties of Paddlewheel Copper(II) Carboxylate Dimers Containing the Ï€â^'Ï€ Stacking, 1,8-Naphthalimide Synthon. Inorganic Chemistry, 2009, 48, 8911-8924. | 4.0 | 94 |
| 13 | Energy conserving approximations to the quantum potential: Dynamics with linearized quantum force. Journal of Chemical Physics, 2004, 120, 1181-1190. | 3.0 | 77 |
| 14 | Absorption Spectrum, Mass Spectrometric Properties, and Electronic Structure of 1,2-Benzoquinone. Journal of Physical Chemistry A, 2010, 114, 7470-7478. | 2.5 | 69 |
| 15 | Geminal model chemistry II. Perturbative corrections. Journal of Chemical Physics, 2004, 120, 10385-10394. | 3.0 | 65 |
| 16 | Semiclassical dynamics based on quantum trajectories. Chemical Physics Letters, 2002, 364, 562-567. | 2.6 | 59 |
| 17 | Geminal model chemistry. IV. Variational and size consistent pure spin states. Journal of Chemical Physics, 2007, 127, 044104. | 3.0 | 57 |
| 18 | Quantum dynamics with Bohmian trajectories: energy conserving approximation to the quantum potential. Chemical Physics Letters, 2003, 376, 358-363. | 2.6 | 56 |

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|---|---|---|---|
| 19 | 6â€31G* basis set for thirdâ€row atoms. Journal of Computational Chemistry, 2001, 22, 976-984. | 3.3 | 56 |
| 20 | Behavior of electronic wave functions near cusps. Journal of Chemical Physics, 1996, 104, 9908-9912. | 3.0 | 50 |
| 21 | The Stable Pentamethylcyclopentadienyl Cation. Angewandte Chemie - International Edition, 2002, 41, 1429-1431. | 13.8 | 49 |
| 22 | 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 |
| 23 | Bohmian dynamics on subspaces using linearized quantum force. Journal of Chemical Physics, 2004, 120, 6815-6825. | 3.0 | 45 |
| 24 | Semiclassical nonadiabatic dynamics with quantum trajectories. Physical Review A, 2005, 71, . | 2.5 | 43 |
| 25 | The relativistic Diracâ€“Coulombâ€“Fock effect on atomization energies. Journal of Chemical Physics, 1999, 110, 7123-7126. | 3.0 | 39 |
| 26 | 1,8-Naphthalimide Synthon in Silver Coordination Chemistry:â€‰ Control of Supramolecular Arrangement. Crystal Growth and Design, 2006, 6, 2758-2768. | 3.0 | 39 |
| 27 | Geminal model chemistry III: Partial spin restriction. Journal of Chemical Physics, 2007, 126, 234112. | 3.0 | 38 |
| 28 | Quantum Trajectory Dynamics in Arbitrary Coordinatesâ€. Journal of Physical Chemistry A, 2006, 110, 5530-5536. | 2.5 | 33 |
| 29 | 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 |
| 30 | Binuclear Aromatic Câ^'H Bond Activation at a Dirhenium Site. Angewandte Chemie - International Edition, 2016, 55, 1324-1327. | 13.8 | 31 |
| 31 | Electron correlation in chemical bonds. Journal of Chemical Physics, 2000, 112, 4014-4019. | 3.0 | 29 |
| 32 | Modified quantum trajectory dynamics using a mixed wave function representation. Journal of Chemical Physics, 2004, 121, 8711-8715. | 3.0 | 29 |
| 33 | Semiclassical nonadiabatic dynamics based on quantum trajectories for the O(P3,D1)+H2 system. Journal of Chemical Physics, 2006, 124, 244307. | 3.0 | 29 |
| 34 | Computational complexity in quantum chemistry. Chemical Physics Letters, 2008, 464, 262-264. | 2.6 | 29 |
| 35 | New operators for electronic density calculation. I. Derivations and formal analysis. Journal of Chemical Physics, 1996, 105, 1470-1478. | 3.0 | 27 |
| 36 | Facile Cï£¿H Bond Formation by Reductive Elimination at a Dinuclear Metal Site. Angewandte Chemie - International Edition, 2014, 53, 11006-11009. | 13.8 | 27 |

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| 37 | 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 |
| 38 | An ab initio linear electron correlation functional. Journal of Chemical Physics, 1999, 110, 3672-3677. | 3.0 | 23 |
| 39 | Semiclassical nonadiabatic dynamics using a mixed wave-function representation. Journal of Chemical Physics, 2005, 123, 174108. | 3.0 | 23 |
| 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 | Local spin from strongly orthogonal geminal wavefunctions. Molecular Physics, 2015, 113, 249-259. | 1.7 | 23 |
| 42 | 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 |
| 43 | 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 |
| 44 | Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Scâ€“Zn. Journal of Chemical Physics, 2008, 128, 144122. | 3.0 | 20 |
| 45 | 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 |
| 46 | Unsaturated Triosmium Carbonyl Cluster Complexes with Bridging Aryl Ligands: Structures, Bonding, and Transformations. Organometallics, 2013, 32, 6368-6378. | 2.3 | 18 |
| 47 | Semiclassical nonadiabatic dynamics of NaFH with quantum trajectories. Chemical Physics Letters, 2007, 446, 395-400. | 2.6 | 15 |
| 48 | 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 |
| 49 | Oxygen Anion Solubility as a Factor in Molten Flux Crystal Growth, Synthesis, and Characterization of Four New Reduced Lanthanide Molybdenum Oxides: Ce<sub>4.918(3)</sub>Mo<sub>3</sub>O<sub>16</sub>, Pr<sub>4.880(3)</sub>Mo<sub>3</sub>O<sub>16</sub>, Nd<sub>4.910(3)</sub>Mo<sub>3</sub>O<sub>16</sub>, and Sm<sub>4.952(3)</sub>Mo<sub>3</sub>O<sub>16</sub>. Crystal Growth and Design, 2016, 16, 4225-4231. | 3.0 | 13 |
| 50 | Spin density in first-row atoms from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1995, 91, 1-15. | 0.8 | 11 |
| 51 | The definition of core electrons. Chemical Physics Letters, 2001, 350, 573-576. | 2.6 | 11 |
| 52 | Synthesis and Transformations of Triosmium Carbonyl Cluster Complexes Containing Bridging Aryl Ligands. Organometallics, 2012, 31, 2961-2964. | 2.3 | 11 |
| 53 | SSpG: A strongly orthogonal geminal method with relaxed strong orthogonality. Journal of Chemical Physics, 2014, 141, 164112. | 3.0 | 11 |
| 54 | Spin density in firstâ€row diatomic hydrides from the Hillerâ€“Sucherâ€“Feinberg identity. Journal of Chemical Physics, 1995, 103, 10058-10069. | 3.0 | 10 |

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| 55 | New operators for calculation of indirect nuclear spinâ€“spin coupling constants. Journal of Chemical Physics, 1997, 107, 5488-5495. | 3.0 | 10 |
| 56 | Semiempirical models for image electrostatics. I. Bare external charge. Journal of Chemical Physics, 2001, 114, 2062-2066. | 3.0 | 10 |
| 57 | Stabilization of Quantum Energy Flows within the Approximate Quantum Trajectory Approach. Journal of Physical Chemistry A, 2007, 111, 10251-10255. | 2.5 | 10 |
| 58 | Dynamic Rotation of Bridging Aryl Ligands in Unsaturated Metal Carbonyl Cluster Complexes. Organometallics, 2013, 32, 1587-1590. | 2.3 | 10 |
| 59 | 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 |
| 60 | Large transition state stabilization from a weak hydrogen bond. Chemical Science, 2020, 11, 7487-7494. | 7.4 | 10 |
| 61 | Lithium atom spin density from the Hiller-Sucher-Feinberg identity. Theoretica Chimica Acta, 1994, 88, 339-349. | 0.8 | 9 |
| 62 | Dynamics in the quantum/classical limit based on selective use of the quantum potential. Journal of Chemical Physics, 2014, 141, 234107. | 3.0 | 9 |
| 63 | Synthesis and Reactivity of Electronically Unsaturated Dirhenium Carbonyl Compounds Containing Bridging Gold-Carbene Groups. Inorganic Chemistry, 2016, 55, 10475-10483. | 4.0 | 9 |
| 64 | The diagonal Bornâ€“Oppenheimer correction to molecular dynamical properties. Chemical Physics Letters, 2001, 333, 459-464. | 2.6 | 8 |
| 65 | Fermi Contact Spin Density Calculations of Aromatic Radicals. Journal of Physical Chemistry C, 2010, 114, 20648-20658. | 3.1 | 8 |
| 66 | Density functional model of multireference systems based on geminals. Chemical Physics Letters, 2012, 543, 205-207. | 2.6 | 8 |
| 67 | Approximate quantum trajectory dynamics for reactive processes in condensed phase. Molecular Simulation, 2015, 41, 86-106. | 2.0 | 7 |
| 68 | Binuclear Aromatic Câ^'H Bond Activation at a Dirhenium Site. Angewandte Chemie, 2016, 128, 1346-1349. | 2.0 | 6 |
| 69 | 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 |
| 70 | Description of electronic excited states using electron correlation operator. Journal of Chemical Physics, 2013, 139, 104111. | 3.0 | 5 |
| 71 | Correlation between the Stability of Substituted Cobaltocenium and Molecular Descriptors. Journal of Physical Chemistry A, 2022, 126, 80-87. | 2.5 | 5 |
| 72 | Analytical potential energy surface for O+C2H2 system. Chemical Physics Letters, 2013, 588, 22-26. | 2.6 | 4 |

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|---|---|---|---|
| 73 | The Stable Pentamethylcyclopentadienyl Cation. Angewandte Chemie - International Edition, 2002, 41, 1642-1642. | 13.8 | 3 |
| 74 | Symmetrization of the nuclear wavefunctions defined by the quantum trajectory dynamics. Theoretical Chemistry Accounts, 2016, 135, 1. | 1.4 | 3 |
| 75 | 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 |
| 76 | 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 |
| 77 | 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 |
| 78 | Description of metals based on localized electrons. Chemical Physics Letters, 2002, 363, 219-225. | 2.6 | 2 |
| 79 | Applicability criterion for semiclassical Bohmian dynamics. International Journal of Quantum Chemistry, 2004, 100, 1057-1064. | 2.0 | 2 |
| 80 | Semiclassical electron correlation operator. Journal of Chemical Physics, 2009, 131, 204102. | 3.0 | 2 |
| 81 | 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 |
| 82 | Molecular dynamics with nuclear quantum effects: Approximations to the quantum force. Annual Reports in Computational Chemistry, 2020, , 41-90. | 1.7 | 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. Journal of Chemical Physics, 2011, 135, 034111. | 3.0 | 1 |
| 86 | Local Measure of Quantum Effects in Quantum Dynamics. Journal of Physical Chemistry A, 2021, 125, 4653-4667. | 2.5 | 1 |
| 87 | 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 |