CURRICULUM VITAE

EDUCATION

University of Notre Dame, Notre Dame, IN **Aug. 1990 - Jan. 1996**

Ph. D. in Chemistry Jan. 1996
M. Sc. in Chemistry May 1992

Moscow Institute of Physics and Technology, Russia **Aug. 1985 - June 1992**

M. Sc. (Magna Cum Laude) June 1992

SCIENTIFIC WORK EXPERIENCE

University of South Carolina, Columbia, SC **professor,** **Jan. 2015 – present**
California Inst. Of Technology, Pasadena, CA **visiting scientist,** **Nov. 2016**
Australian National University, Canberra Australia **visiting scientist,** **May-June 2016**
University of South Carolina, Columbia, SC **associate professor,** **June 2007 –Dec. 2014**
University of South Carolina, Columbia, SC **assistant professor,** **Aug. 2001 - June 2007**

- C-H bond activation: Computational studies of late transition metal clusters
- Correlation operator: Description of electron correlation effects using 2-electron operators and single determinant wavefunctions.
- Geminal Theory: Building model chemistries based on antisymmetric product of electron pairs.
- Semiclassical Bohmian dynamics: Development of computationally cheap method to capture leading quantum corrections to nuclear dynamics.

Northwestern University, Evanston, IL **postdoctoral fellow, Feb. 1996 - Aug. 2001**

- Correlation operator: Analysis of the possibilities and shortcomings of widely popular Density Functional Theory led us to the description of correlation effects via correlation operator. We found it to work well for atoms, and try to apply correlation operator approach for molecules.

- Image potential: How does the force between the metal surface and the approaching charge gets modified from its classical form when two are close enough to interact? We develop a Pariser-Parr-Pople type model of a metal to investigate this question computationally.

- Born-Oppenheimer correction: The quantum motion of nuclei may have an important contribution to the precise thermochemical calculations and to the height and shape of reaction barriers. We investigate both types of effects by refining a Born-Oppenheimer theory, and doing thermochemical analysis and the reaction dynamics.

- G3 theory: A very accurate thermochemical calculations can be performed on a medium-sized (~100 electrons) molecules by using the Gaussian-3 theory. We help to extend the theory to third-row elements and refine it by analyzing relativistic and Born-Oppenheimer contributions, and developing new basis sets.

University of Notre Dame, Notre Dame, IN **research assistant, Sept. 1992 - Jan. 1996**

The analysis of electron spin and nuclear magnetic resonance spectra often requires a computational input. The computations use a delta function operator that is difficult to get with satisfactory precision. We developed a new class of operators which, being computationally almost as efficient as the delta function, significantly improved calculations of spin densities on nuclei. In the analysis of new operators we discovered a number of general mathematical theorems useful in wave function computations.

University of Notre Dame, Notre Dame, IN **research assistant, Aug. 1990 - Dec. 1991**

Many properties of the ionized liquids and solids can be determined by knowing the distribution of distances between the parent cations and thermalized electrons. We used a Monte-Carlo simulation to obtain and rationalize the distribution of thermalized electrons in liquid hydrocarbons.

Institute of Energy Problems in Chemical Physics, Chernogolovka, Russia **research assistant, Sept. 1989- May 1990**

We measured recombination parameters of photoexcited electrons in n-hexane. The data was found to be consistent with Mozumder-Magee model of electron energy loss in non-polar media.

TEACHING EXPERIENCE

University of South Carolina

CHEM 743 "Quantum Chemistry" course	2001 – 2015, 11 times
CHEM 541 "Physical Chemistry I" course	2003 – 2017, 9 times
CHEM 542 "Physical Chemistry II" course	2012, once
CHEM 142 "Honors General Chemistry II" course	2018, once
CHEM 112 "General Chemistry II" course	2004 – 2015, 10 times

University of Notre Dame

Teaching Assistant for undergraduate Physical Chemistry	fall 1992
Teaching Assistant for General Chemistry Lab	fall 1990, spring 1991

RESEARCH SUPERVISION

University of South Carolina

Post-graduate supervision

Sophya V. Garashchuk, research assistant professor	09/2001 – 08/2008
Guangcan Yang, postdoc	10/2003 – 11/2004
Khaled Bahloul, postdoc	11/2003 – 11/2004

Graduate supervision

Feng Xu	08/2003 – 12/2007
Liyan Liang	08/2004 – 05/2011
Sonali Mitra	08/2008 – 10/2009
Brett Cagg	09/2011 – 08/2015
Bryan Nichols	11/2011 – 01/2015
Shehani Wettasinghe	11/2017 – current

Undergraduate supervision

Ry Ely, REU student	06/2002 – 08/2002
Ben Garrett	05/2007 – 08/2007
Clifford Weir, summer research	06/2009 – 07/2009

HONORS AND AWARDS

Invited Professor, University of Nice, France	11/2009 – 12/2009
IBM-Lowdin fellowship, 44th Sanibel Symposium	2004
Finalist in the ACS symposium on emerging technologies in comp. chemistry	2002

PUBLICATIONS

Articles

77. Albarran G, Rassolov VA, Schuler RH. **2018** OH Radical as a Probe of the Spin Polarizability in 1-and 2-Naphthol, *JOURNAL OF PHYSICAL CHEMISTRY A* 122(16) 4015-4022, 10.1021/acs.jpca.7611718
76. Kittikhunnatham P, Som B, Rassolov V, Stolte M, Wurthner F, Shimizu LS, Greytak AB. **2017** 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*, 121(33): 18102-18109, 10.1021/acs.jpcc.7b07136
75. Gu B, Rassolov VA, Garashchuk S. **2016** Symmetrization of the nuclear wavefunctions defined by the quantum trajectory dynamic, *THEORETICAL CHEMISTRY ACCOUNTS* 135(12): 267(1-13)
74. Adams RD, Dhull P, Rassolov V, Wong YO. **2016** Synthesis and Reactivity of Electronically Unsaturated Dirhenium Carbonyl Compounds Containing Bridging Gold-Carbene Groups, *INORGANIC CHEMISTRY* 55(20): 10475-10483
73. Cortese AJ, Abeysinghe D, Wilkins B, Smith MD, Rassolov V, zur Loye HC. **2016** Oxygen Anion Solubility as a Factor in Molten Flux Crystal Growth, Synthesis, and Characterization of Four New Reduced Lanthanide Molybdenum Oxides: $Ce_{4.918(3)}Mo_3O_{16}$, $Pr_{4.880(3)}Mo_3O_{16}$, $Nd_{4.910(3)}Mo_3O_{16}$, and $Sm_{4.952(3)}Mo_3O_{16}$, *CRYSTAL GROWTH & DESIGN* 16(8): 4225-4231
72. Adams RD, Luo ZW, Chen MW, Rassolov VA. **2016** Multicenter transformations of the methyl ligand in CH_3Os_3Au carbonyl cluster complexes: Synthesis, characterization and DFT analyses, *JOURNAL OF ORGANOMETALLIC CHEMISTRY* 812(SI): 95-107
71. Adams RD, Rassolov V, Wong YO. **2016** Binuclear Aromatic C-H Bond Activation at a Dirhenium Site, *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 55(4): 1324-1327
70. Gu B,Hinde RJ, Rassolov VA, Garashchuk SG **2015** Estimation of the Ground State Energy of an Atomic Solid by Employing Quantum Trajectory Dynamics with Friction *J. CHEM. THEO. COMP*. 11(7): 2891-2899
69. Shao YH; Gan ZT; Epifanovsy E et al **2015** Advances in molecular quantum chemistry contained in the Q-Chem 4 program package *MOLECULAR PHYSICS* 113 (2): 184-215
68. Garashchuk SG, Jakowski J, Rassolov VA. **2015** Approximate quantum trajectory dynamics for reactive processes in condensed phase, *MOLECULAR SIMULATION* 41(1-3): 86-106
67. Jeszenszki P, Rassolov VA, Surjan P, Szabados A **2015** Local spin from strongly orthogonal germinal wavefunctions, *MOLECULAR PHYSICS* 113 (3-4): 249-259
66. Adams RD, Rassolov V, Wong YO. **2014** Facile C-H Bond Formation by Reductive Elimination at a Dinuclear Metal Site, *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 53(41): 11006-11009
65. Cagg BA, Rassolov VA. **2014** SS(p)G: A strongly orthogonal geminal method with relaxed strong orthogonality, *J. CHEM. PHYS*. 141(16): 164112
64. Garashchuk SG, Dell'Angelo D, Rassolov VA. **2014** Dynamics in the quantum/classical limit based on selective use of the quantum potential *J. CHEM. PHYS*. 141(23): 234107
63. Adams RD, Rassolov V, Zhang Q. **2013** Unsaturated Triosmium Carbonyl Cluster Complexes with Bridging Aryl Ligands: Structures, Bonding, and Transformations, *ORGANOMETALLICS* 32(21): 6368-6378
62. Garashchuk S, Rassolov V, Braams BJ. **2013** Analytical potential energy surface for $O+C_2H_2$ system, *CHEMICAL PHYSICS LETTERS* 588: 22-26
61. Nichols B, Rassolov VA. **2013** Description of electronic excited states using electron correlation operator, *JOURNAL OF CHEMICAL PHYSICS* 139(10): 104111
60. Adams RD, Kan Y, Rassolov V, et al. **2013** Tetraruthenium carbonyl complexes containing germyl and stannyl ligands from the reactions of Ru-4(CO)(13)(mu-H)(2) with HGePh3 and HSnPh3, *JOURNAL OF ORGANOMETALLIC CHEMISTRY*: 20-31
59. Adams RD, Rassolov V, Zhang Q. **2013** Dynamic Rotation of Bridging Aryl Ligands in Unsaturated Metal Carbonyl Cluster Complexes, *ORGANOMETALLICS* 32(6): 1587-1590
58. Cagg BA, Rassolov VA. **2012** Density functional model of multireference systems based on geminals *CHEMICAL PHYSICS LETTERS* 543: 205-207
57. Adams RD , Rassolov V, Zhang Q. **2012** Synthesis and Transformations of Triosmium Carbonyl Cluster Complexes Containing Bridging Aryl Ligands *ORGANOMETALLICS* 31(8): 2961-2964
56. Rassolov VA. **2011** Harmonic electron correlation operator *JOURNAL OF CHEMICAL PHYSICS* 135(3): 0341112
55. Liang L, Rassolov VA. **2010** Fermi Contact Spin Density Calculations of Aromatic Radicals . *JOURNAL OF PHYSICAL CHEMISTRY C* 114(48): 20648-20658
54. Albarran G, Boggess W, Rassolov V, Schuler RH. **2010** Absorption Spectrum, Mass Spectrometric Properties, and Electronic Structure of 1,2-Benzoquinone . *JOURNAL OF PHYSICAL CHEMISTRY A* 114(28): 7470-7478

53. Cassam-Chenai P, Rassolov V. **2010** The electronic mean field configuration interaction method: III - the p-orthogonality constraint *CHEMICAL PHYSICS LETTERS* 487(1-3): 147-152
52. Rassolov VA **2009** Semiclassical electron correlation operator *JOURNAL OF CHEMICAL PHYSICS* 131(20): 204102
51. Reger DL, Debreczeni A, Reinecke B, Rassolov V, Smith MD. **2009** Highly Organized Structures and Unusual Magnetic Properties of Paddlewheel Copper(II) Carboxylate Dimers Containing the pi-pi Stacking, 1,8-Naphthalimide Synthon *INORGANIC CHEMISTRY* 48(18): 8911-8924
50. Bharathy M, Rassolov, VA, Park S, zur Loye HC. **2008** Crystal growth of Two New Photoluminescent Oxides: $Sr_3Li_6Nb_2O_{11}$ and $Sr_3Li_6Ta_2O_{11}$ *INORGANIC CHEMISTRY* 47(21): 9941-9945
49. Rassolov VA, Garashchuk S. **2008** Computational complexity in quantum chemistry *CHEMICAL PHYSICS LETTERS* 464 (4-6): 262-264
48. Garashchuk S, Rassolov VA. **2008** Stable long-time semiclassical description of zero-point energy in high-dimensional molecular systems *JOURNAL OF CHEMICAL PHYSICS* 129 (2): 024109
47. Roof IP, Park S, Vogt T, Rassolov V, Smith MD, Omar S, Nino J, zur Loye HC. **2008** Crystal growth of two new niobates, La_2KNbO_6 and Nd_2KNbO_6: Structural, dielectric, photophysical, and photocatalytic properties *CHEMISTRY OF MATERIALS* 20(10): 3327-3335
46. Mayhall NJ, Raghavachari K, Redfern PC, Curtiss LA , Rassolov VA. **2008** Toward accurate thermochemical models for transition metals: G3Large basis sets for atoms Sc-Zn *JOURNAL OF CHEMICAL PHYSICS* 128(14): 144122
45. Bharathy M, Rassolov VA, zur Loye HC**. 2008** Crystal growth of Sr_3NaNbO_6 and Sr_3NaTaO_6: New photoluminescent oxides *CHEMISTRY OF MATERIALS* 20(6): 2268-2273
44. Garashchuk S, Rassolov VA. **2007** Semiclassical nonadiabatic dynamics of NaFH with quantum trajectories. *CHEMICAL PHYSICS LETTERS* Volume: 446 (4-6): 395-400
43. Garashchuk S, Rassolov VA. **2007** Stabilization of quantum energy flows within the approximate quantum trajectory approach. *JOURNAL OF PHYSICAL CHEMISTRY A* 111(41): 10251-10255
42. Rassolov VA, Xu F. **2007** Geminal model chemistry. IV. Variational and size consistent pure spin states *JOURNAL OF CHEMICAL PHYSICS* 127(4): 044104
41. Rassolov VA, Xu F. **2007** Geminal model chemistry III: Partial spin restriction *JOURNAL OF CHEMICAL PHYSICS* 126 (23): 234112
40. Reger, DL; Semeniuc, RF; Elgin JD; Rassolov V; Smith MD. **2006** 1,8-naphthalimide synthon in silver coordination chemistry: Control of supramolecular arrangement *CRYSTAL GROWTH & DESIGN* 6(12): 2758-2768
39. Garashchuk, S; Rassolov, VA; Schatz, GC. **2006** Semiclassical nonadiabatic dynamics based on quantum trajectories for the $O(^3P,^1D)+H_2$ system.*JOURNAL OF CHEMICAL PHYSICS* 124 (24): 244307 (8 pages)
38. Shao, Y;Molnar, LF; Jung, Y; Kussmann, J;Ochsenfeld, C; Brown, ST;Gilbert, ATB; Slipchenko, LV; Levchenko, SV; O'Neill, DP; Distasio, RA;Lochan, RC; Wang, T; Beran, GJO; Besley, NA; Herbert, JM; Lin, CY; Van Voorhis, T; Chien, SH; Sodt, A; Steele, RP; Rassolov, VA; Maslen, PE; Korambath, PP; Adamson, RD; Austin, B; Baker, J; Byrd, EFC; Dachsel, H; Doerksen, RJ; Dreuw, A; Dunietz, BD; Dutoi, AD; Furlani, TR; Gwaltney, SR; Heyden, A; Hirata, S; Hsu, CP; Kedziora, K; Khalliulin, RZ; Klunzinger, P; Lee, AM; Lee, MS; Liang, WZ; Lotan, I; Nair, N; Peters, B; Proynov, EI; Pieniazek, PA; Rhee, YM; Ritchie, J; Rosta, E; Sherrill, CD; Simmonett, AC; Subotnik, JE; Woodcock, HL; Zhang, W; Bell, AT; Chakraborty, AK; Chipman, DM; Keil, FJ; Warshel, A; Hehre, WJ; Schaefer III, HF; Kong, J;Krylov, AI; Gill, PMW; Head-Gordon, M. **2006** Advances in methods and algorithms in a modern quantum chemistry program package *PHYSICAL CHEMISTRY CHEMICAL PHYSICS* 8 (27): 3172-3191
37. Rassolov, VA; Garashchuk, S; Schatz, GC. **2006** Quantum trajectory dynamics in arbitrary coordinates *JOURNAL OF PHYSICAL CHEMISTRY A* 110 (16): 5530-5536
36. Garashchuk, S; Rassolov, VA; Schatz, GC. **2005** Semiclassical nonadiabatic dynamics using a mixed wave-function representation.*JOURNAL OF CHEMICAL PHYSICS* 123 (17): 174108 (10 pages)
35. Rassolov, VA; Garashchuk, S. **2005** Semiclassical nonadiabatic dynamics with quantum trajectories *PHYSICAL REVIEW A* 71 (3): 032511 (10 pages)
34. Garashchuk, S; Rassolov, VA. **2004** Applicability criterion for semiclassical Bohmian dynamics *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY* 100 (6): 1057-1064
33. Garashchuk, S; Rassolov, VA. **2004** Modified quantum trajectory dynamics using a mixed wave function representation *JOURNAL OF CHEMICAL PHYSICS* 121 (18): 8711-8715
32. Rassolov, VA; Xu, F; Garashchuk, S. **2004** Geminal model chemistry II. Perturbative corrections *JOURNAL OF CHEMICAL PHYSICS* 120 (22): 10385-10394
31. Rassolov, VA; Garashchuk, S. **2004** Bohmian dynamics on subspaces using linearized quantum force *JOURNAL OF CHEMICAL PHYSICS* 120 (15): 6815-6825
30. Reger, DL; Semeniuc, RF; Rassolov, V; Smith, MD. **2004** Supramolecular structural with changes in anion and solvent in silver(I) complexes of a semirigid, bitopic tris(pyrazolyl)methane ligand *INORGANIC CHEMISTRY* 43 (2): 537-554
29. Garashchuk, S; Rassolov, VA. **2004** Energy conserving approximations to the quantum potential: Dynamics with linearized quantum force *JOURNAL OF CHEMICAL PHYSICS* 120 (3): 1181-1190
28. Garashchuk, S; Rassolov, VA. **2003** Quantum dynamics with Bohmian trajectories: energy conserving approximation to the

quantum potential *CHEMICAL PHYSICS LETTERS* 376 (3-4): 358-363

27. Garashchuk, S; Rassolov, VA. **2003** Semiclassical dynamics with quantum trajectories: and comparison with the semiclassical initial value representation propagator *JOURNAL OF CHEMICAL PHYSICS* 118 (6): 2482-2490 (In Print)
26. Garashchuk, S; Rassolov, VA. **2002** Semiclassical dynamics based on quantum trajectories *CHEMICAL PHYSICS LETTERS* 364 (5-6): 562-567
25. Rassolov, VA. **2002** A geminal model chemistry *JOURNAL OF CHEMICAL PHYSICS* 117 (13): 5978-5987
24. Rassolov, VA; Garashchuk, SV; Ratner, MA. **2002** Description of metals based on localized electrons *CHEMICAL PHYSICS LETTERS* 363 (3-4): 219-225

23a. Lambert, JB; Lin, LJ; Rassolov, V. **2002** The stable pentamethylcyclopentadienyl cation (vol 41, pg 1429, 2002) *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 41 (10): 1642-1642

23. Lambert, JB; Lin, LJ; Rassolov, V. **2002** The stable pentamethylcyclopentadienyl cation *ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 41 (8): 1429-1431
22. Rassolov, VA; Pople, JA; Redfern, PC; Curtiss, LA. **2001** The definition of core electrons *CHEMICAL PHYSICS LETTERS* 350 (5-6): 573-576
21. Curtiss, LA; Redfern, PC; Rassolov, V; Kedziora, G; Pople, JA. **2001** Extension of Gaussian-3 theory to molecules containing third-row atoms K, Ca, Ga-Kr *JOURNAL OF CHEMICAL PHYSICS* 114 (21): 9287-9295
20. Rassolov, VA; Ratner, MA; Pople, JA; Redfern, PC; Curtiss, LA. **2001** 6-31G* basis set for third-row atoms *JOURNAL OF COMPUTATIONAL CHEMISTRY* 22 (9): 976-984
19. Rassolov, VA; Mozumder, A. **2001** Monte Carlo simulation of electron thermalization distribution in liquid hydrocarbons: Effects of inverse collisions and of an external electric field *JOURNAL OF PHYSICAL CHEMISTRY B* 105 (7): 1430-1437
18. Rassolov, VA; Ratner, MA; Pople, JA. **2001** Semiempirical models for image electrostatics. I. Bare external charge *JOURNAL OF CHEMICAL PHYSICS* 114 (5): 2062-2066
17. Garashchuk, S; Light, JC; Rassolov, VA. **2001** The diagonal Born-Oppenheimer correction to molecular dynamical properties *CHEMICAL PHYSICS LETTERS* 333 (6): 459-464
16. Kong, J; White, CA; Krylov, AI; Sherrill, D; Adamson, RD; Furlani, TR; Lee, MS; Lee, AM; Gwaltney, SR; Adams, TR; Ochsenfeld, C; Gilbert, ATB; Kedziora, GS; Rassolov, VA; Maurice, DR; Nair, N; Shao, YH; Besley, NA; Maslen, PE; Dombroski, JP; Daschel, H; Zhang, WM; Korambath, PP; Baker, J; Byrd, EFC; Van Voorhis, T; Oumi, M; Hirata, S; Hsu, CP; Ishikawa, N; Florian, J; Warshel, A; Johnson, BG; Gill, PMW; Head-Gordon, M; Pople, JA. **2000** Q-Chem 2.0: A high-performance ab initio electronic structure program package *JOURNAL OF COMPUTATIONAL CHEMISTRY* 21 (16): 1532-1548
15. Rassolov, VA; Pople, JA; Ratner, MA. **2000** Reply to "Comment on 'Correlation holes in a spin-polarized dense electron gas'" *PHYSICAL REVIEW B* 62 (3): 2232-2235
14. Rassolov, VA; Ratner, MA; Pople, JA. **2000** Electron correlation in chemical bonds *JOURNAL OF CHEMICAL PHYSICS* 112 (9): 4014-4019
13. Rassolov, VA; Pople, JA; Ratner, MA. **1999** Correlation holes in a spin-polarized dense electron gas *PHYSICAL REVIEW B* 59 (24): 15625-15631
12. Kedziora, GS; Pople, JA; Rassolov, VA; Ratner, MA; Redfern, PC; Curtiss, LA. **1999** The relativistic Dirac-Coulomb-Fock effect on atomization energies *JOURNAL OF CHEMICAL PHYSICS* 110 (15): 7123-7126
11. Curtiss, LA; Redfern, PC; Raghavachari, K; Rassolov, V; Pople, JA. **1999** Gaussian-3 theory using reduced Moller-Plesset order *JOURNAL OF CHEMICAL PHYSICS* 110 (10): 4703-4709
10. Rassolov, VA. **1999** An ab initio linear electron correlation functional *JOURNAL OF CHEMICAL PHYSICS* 110 (8): 3672-3677
9. Curtiss, LA; Raghavachari, K; Redfern, PC; Rassolov, V; Pople, JA. **1998** Gaussian-3 (G3) theory for molecules containing first and second-row atoms *JOURNAL OF CHEMICAL PHYSICS* 109 (18): 7764-7776
8. Rassolov, VA; Pople, JA; Ratner, MA; Windus, TL. **1998** 6-31G* basis set for atoms K through Zn *JOURNAL OF CHEMICAL PHYSICS* 109 (4): 1223-1229
7. Chipman, DM; Rassolov, VA. **1997** New operators for calculation of indirect nuclear spin-spin coupling constants *JOURNAL OF CHEMICAL PHYSICS* 107 (14): 5488-5495
6. Rassolov, VA; Chipman, DM. **1996** New operators for electronic density calculation .1. Derivations and formal analysis *JOURNAL OF CHEMICAL PHYSICS* 105 (4): 1470-1478
5. Rassolov, VA; Chipman, DM. **1996** New operators for electronic density calculation .2. Application to hydrogen, first-row atoms, and first-row diatomic hydrides *JOURNAL OF CHEMICAL PHYSICS* 105 (4): 1479-1491
4. Rassolov, VA; Chipman, DM. **1996** Behavior of electronic wave functions near cusps *JOURNAL OF CHEMICAL PHYSICS* 104 (24): 9908-9912
3. Rassolov, VA; Chipman, DM. **1995** Spin-density in first-row diatomic hydrides from the Hiller-Sucher-Feinberg identity *JOURNAL OF CHEMICAL PHYSICS* 103 (23): 10058-10069
2. Rassolov, VA; Chipman, DM. **1995** Spin-density in first-row atoms from the Hiller-Sucher-Feinberg identity *THEORETICA CHIMICA ACTA* 91 (1-2): 1-15

1. Rassolov, VA; Chipman, DM. **1994** Lithium atom spin-density from the Hiller-Sucher-Feinberg identity *THEORETICA CHIMICA ACTA* 88 (5): 339-349

book chapters

V. Rassolov and S. Garashchuk, in "**Quantum Trajectories**", Semiclassical Implementation of Bohmian Dynamics, P. Chattaraj (Ed), CRC Press, 2011

S. Garashchuk,V. Rassolov, and O. Prezhdo in "**Reviews of Computational Chemistry**", vol. 27, Semiclassical Bohmian Dynamics, K. Lopkowitz (Ed), Wiley, 2011

V. Rassolov and D. Chipman, in **Calculation of NMR and EPR Parameters: Theory and Application**, Chapter 31, Alternative Fermi Contact operators for EPR and NMR , p 493-504 (Wiley, 2004)

PRESENTATIONS

Invited

Geminal model chemistries, **Nov 2016** at theory seminar, U. of Southern California
Geminal model chemistries, **Nov 2016** at Tom Miller group, Caltech
Electron Correlation Operator Approach for Description of Excited States, **July 2015** at the workshop: Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, Telluride CO
Quantum Chemistry from Os Au carbonyl clusters to electron correlation operators, **Nov 2013** at Syracuse University, Syracuse, NY
Quantum Chemistry from Os Au carbonyl clusters to electron correlation operators, **Oct 2013** at Francis Marion University, Florence, SC
Multireference DFT, **Aug 2013** at VII Congress of Theoretical Chemical Physics, Budapest, Hungary
Mixed Quantum-Classical Dynamics in Bohmian Formulation, **July 2013** at the workshop: Quantum Trajectories: Foundations and Future, Telluride CO
Quantum Chemistry from Os Au carbonyl clusters to electron correlation operators, **Feb 2013** at Tulane University, New Orleans LA
Harmonic correlation operator, **May 2012** at the 41th Southeast Theoretical Chemistry Association Meeting at the University of Georgia, Athens GA
Geminal model chemistries, **Nov 2011** at Wake Forest University, NC
Geminal model chemistries, **Mar 2010** at the 50th Sanibel Symposium, St. George Island, GA
Semiclassical Bohmian Dynamics, **Dec 2009** at the Laboratoire de mathematiques J. A. Dieudonne, Universite de Nice Sophia-Antipolis, Nice, France
Semiclassical correlation operator, **May 2009** at the 38th Southeast Theoretical Chemistry Association Meeting at Duke University, NC
Stable Long-time semiclassical Description of Zero-point Energy in High-dimensional Molecular Systems, **Jan 2009** at the workshop "Chemical Dynamcs: Challenges and Approaches", Minneapolis, MN
Stable Long-time semiclassical Description of Zero-point Energy in High-dimensional Molecular Systems, **Sep 2008** at Theory and Applications of Computational Chemistry, Shanghai, China
Polynomial Scaling of Spin Problem, **Sep 2008** at World Association of Theoretical and Computational Chemists meeting, Sydney, Australia
Computational Complexity of Non-relativistic Quantum Mechanics: Implications for the Quantum Potential, **Jul 2008** at the Workshop on Quantum Trajectories, Los Alamos, NM
Polynomial Scaling of Spin Problem, **July 2008** at the VI Congress of the International Society for Theoretical Chemical Physics, Vancouver Canada
Geminals as wavefunctions building blocks: New level of model chemistry, **Oct 2007** at the workshop on mathematical methods in chemistry, Nice, France
Long-time stable semiclassical dynamcs, **Dec 2006** at the Workshop on Bohmian Dynamics, Ausin, TX
Semiclassical dynamics employing approximate quantum potential, **June 2006** at the 2006 Great Lakes Regional ACS Meeting in Milwaukee, WI
Semiclassical nonadiabatic dynamics with quantum trajectories, **August 2005** at the 230th National ACS Meeting in Washington, DC
Semiclassical nonadiabatic dynamics in mixed representation, **May 2005** at the 34th Southeast Theoretical Chemistry Association Meeting in Knoxville, TN
Recent developments in geminal model chemistries, **March 2005** at the 229th National ACS Meeting in San Diego, CA
Non-locality and non-classical momentum in semiclassical Bohmian dynamics. The density nodes, **July 2004** at the workshop

"Quantum and Semiclassical molecular dynamics of nanostructures" in Los Alamos, NM
A geminal model chemistry, **May 2003** at the 2003 Great Lakes Regional ACS Meeting in Chicago, IL
Model chemistry based on strongly orthogonal geminals, **March 2003** at the 225th National ACS Meeting in New Orleans, LA
Model chemistry based on electron geminals, **January 2003** at the Quantum Los Alamos National Laboratory, Los Alamos, NM (seminar)
Geminal model chemistry, **December 2002** at the Quantum Theory Project at the University of Florida, Gainesville, FL (seminar)
Geminal model chemistry, **April 2002** at the Center for Computational Quantum Chemistry at the University of Georgia, Athens, GA (seminar)

Contributed

More than 10 contributed talks in the last 5 years

FUNDING

South Carolina Computational Chemistry Consortium (SC4), SC EPSCOR $ 117,311 06/13 - 07/14

Development of correlation operator approach to model electron correlation, NSF $ 220,000, 07/12 - 06/16

Computer cluster for wide range chemical applications and Education, PI: Dawson, Co-PI: Adams, Garashchuk, Rassolov, Shimizu, NSF, $220,550, 01/01/11-12/31/13

Computational Chemistry Workshop, SC EPSCOR $ 4,995 05/12 - 09/12

Development of partially spin-restricted geminal model for studies of transition metal compounds, Petroleum Research Fund, $ 80,000, 09/01/06-08/31/10

Semiclassical dynamics and description of nonadiabatic effects, NSF $ 311,000, 09/01/05-08/31/09

SGER: Model Chemistry Based on Electron Geminals, NSF, $ 92,804, 06/01/03-05/31/04

Multidimensional Semiclassical Dynamics with Quantum Trajectories, Petroleum Research Fund, $ 35,000, 09/01/02-08/31/05

Modeling of Interactions between Charges and Nanoparticle, Research and Productive Scholarships, USC, $14,500, 04/01/02-06/30/03