GERGELY GIDOFALVI

DEPARTMENT OF CHEMISTRY AND BIOCHEMSITRY
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EDUCATION

Ph.D. in Chemistry, University of Chicago	August 2006
M.S. in Chemistry, University of Chicago	March 2003
B.S. in Chemistry, Summa Cum Laude, San Diego State University	May 2002

ACADEMIC APPOINTMENTS

Associate Professor, Department of Chemistry and Biochemistry Gonzaga University	2016 – present
Assistant Professor, Department of Chemistry and Biochemistry Gonzaga University	2010 – 2016

PROFESSIONAL EXPERIENCE

Postdoctoral Fellow, Argonne National Laboratory	2007 – 2010
Postdoctoral Fellow, University of Chicago	2006 – 2007

DISTINCTIONS/AWARDS

Director's Postdoctoral Fellowship	Argonne National Laboratory, 2007 – 2009
Yang Cao-Lan-Xian Best Thesis Award	Dept. of Chemistry, University of Chicago, 2006
Physical Sciences Teaching Prize	Physical Sciences Collegiate Division and Physical Sciences Division, University of Chicago, 2004
Graduate Research Fellowship	National Science Foundation, 2003 – 2006
McCormick Fellowship	Dept. of Chemistry, University of Chicago, 2002 – 2003

EXTERNAL FUNDING

"Parallel Two-Electron Reduced-Density-Matrix-Based Electronic Structure Software For Highly Correlated Molecules and Materials", Department of the Army, 2016-2018, $34,629. Submitted on 3/10/2016. Role: co-PI.

"Orbital optimization and excited-state calculation within the graphically contracted function method", Research Corporation, 2011-2013, $45,364. Submitted/11/15/2011. Role: PI.

PUBLICATIONS (* indicates GU undergraduate)

- J. Fosso-Tande, T.-S. Nguyen*, **G. Gidofalvi**, and A. E. DePrince III, J. Chem. Theor. and Comp., **12**, 2260-2271 (2016). *"Large-scale Variational Two-Electron Reduced-Density-Matrix-Driven Complete Active Space Self-Consistent Field Methods"*
- R. Shepard, S. R. Brozell, and **G. Gidofalvi**, *J. Phys. Chem A* **119**, 7924 (2015).*"The representation and parameterization of orthogonal matrices"*
- Evan Jahrman*, Proceedings Of the National Conference on Undergraduate Research 2014. *"The use of natural orbitals in predicting molecular properties"* http://www.ncurproceedings.org/ojs/index.php/NCUR2014/article/view/1034
- **G. Gidofalvi**, S. R. Brozell, and R. Shepard, *Theor. Chem. Acc.* **133**, 1512 (2014). *"Wave function analysis with Shavitt graph density in the graphically contracted function method"*
- R. Shepard, **G. Gidofalvi**, and S. R. Brozell, *J. Chem. Phys.* **141**, 064106 (2014).*"The graphically contracted function method: II A general procedure for the parameterization of orthogonal matrices and its application to arc factors"*
- R. Shepard, **G. Gidofalvi**, and S. R. Brozell, *J. Chem. Phys.* **141**, 064105 (2014).*"The graphically contracted function method: I Formulation and implementation"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Phys. Chem. A* **118**, 495 (2014). "*Molecule-optimized basis sets and Hamiltonians for accelerated electronic structure calculations of atoms and molecules"*
- P. G. Szalay, T. Müller, **G. Gidofalvi**, H. Lischka, and R. Shepard, *Chem. Rev.* **112**, 108 (2012). "*Multiconfiguration self-consistent field and multireference configuration interaction methods and applications"*
- K. Pelzer, L. Greenman, **G. Gidofalvi**, and D. A. Mazziotti, *J. Phys. Chem. A* **115,** 5632 (2011). *"Strong correlation in acene sheets from the active-space variational two-electron reduced density matrix method: effects of symmetry and size"*
- **G. Gidofalvi** and R. Shepard, *Mol. Phys.* **108**, 2717 (2010). *"Exploiting sparsity in the graphically contracted function configuration interaction method"*
- R. Shepard, **G. Gidofalvi**, and P. D. Hovland, *Int. J. Quantum Chem.* **110**, 2938 (2010). *"An efficient recursive algorithm to compute wave function optimization gradients for the graphically contracted function method"*
- **G. Gidofalvi**, R. Shepard, *Int. J. Quantum Chem.* **109**, 3552 (2009). *"The evaluation of spin density matrices within the graphically contracted function method"*
- **G. Gidofalvi**, R. Shepard, *J. Comp. Chem.* **30**, 2414 (2009).*"Computation of determinant expansion coefficients within the graphically contracted function method"*
- **G. Gidofalvi**, D. A. Mazziotti, *Phys. Rev. A* **80**, 022507 (2009). "*Direct calculation of excited-state electronic energies and two-electron reduced density matrices from the anti-Hermitian contracted Schrödinger equation"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Chem. Phys.* **129**, 134108 (2008). *"Active-space two-electron reduced-density-matrix method: complete active-space calculations without diagonalization of the N-electron Hamiltonian"*

- **G. Gidofalvi**, D. A. Mazziotti, *J. Chem. Phys.* **127**, 244105 (2007). "*Multireference self-consistent field energies without the many-electron wavefunction through a variational low-rank two electron reduced-density-matrix method"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Chem. Phys.* **126**, 024105 (2007). "*Molecular properties from variational reduced-density-matrix theory with three-particle N-representability conditions"*
- **G. Gidofalvi**, and D. A. Mazziotti, *J. Chem. Phys. **125**, 144102 (2006). "Computation of dipole, quadrupole, and octupole surfaces from the variational two-electron reduced density matrix method"*
- **G. Gidofalvi**, D. A. Mazziotti, *Phys. Rev. A* **74**, 012501 (2006). *"Computation of quantum phase transitions by reduced-density-matrix mechanics"*
- J. D. Farnum, **G. Gidofalvi**, and D. A. Mazziotti, *J. Chem. Phys.* **124**, 234103 (2006). *"Modeling the influence of a laser pulse on the potential energy surface in optimal molecular control theory"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Phys. Chem. A* **110**, 5481 (2006).*"Variational reduced-density matrix theory applied to the potential energy surfaces of carbon monoxide in the presence of electric fields"*
- **G. Gidofalvi**, D. A. Mazziotti, *Phys. Rev. A* **72**, 052505 (2005).*"Spin and symmetry adaptation of the variational two-electron reduced-density-matrix method"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Chem. Phys.* **122,** 194104 (2005).*"Application of variational reduced-density-matrix theory to the potential energy surfaces of the nitrogen and carbon dimers"*
- **G. Gidofalvi**, D. A. Mazziotti, *J. Chem. Phys.* **122,** 094107 (2005). "*Application of variational reduced-density-matrix theory to organic molecules"*
- **G. Gidofalvi**, D. A. Mazziotti, *Chem. Phys. Lett.* **398**, 434 (2004). *"Variational reduced-density matrix theory: strength of Hamiltonian-dependent positivity conditions"*
- **G. Gidofalvi**, D. A. Mazziotti, *Phys. Rev. A* **69,** 042511 (2004). "*Boson correlation energies via variational minimization with the two-particle reduced density matrix: Exact N-representability conditions for harmonic interactions"*
- **G. Gidofalvi**, C. F. Wong, and J. A. McCammon, *J. Chem. Ed.* **79**, 1122 (2002). "*Entropy loss of hydroxyl groups of balanol upon binding to protein kinase A"*

INVITED TALKS

- **242nd National Meeting of the American Chemical Society**, Reduced Density Matrices in Quantum Chemistry and Physics Symposium, 2011, Denver, CO. "*Applications of variational 2-RDM theory to strongly correlated systems*"
- **Argonne National Laboratory Postdoctoral Symposium**, 2009, Argonne National Laboratory, Argonne IL. "*Evaluation of determinant expansion coefficients and spin density matrices within the graphically contracted function method"*
- **238th National Meeting of the American Chemical Society**, Postdoctoral Research Highlights Symposium, 2009, Washington, DC. "*Evaluation of determinant expansion coefficients and spin density matrices within the graphically contracted function method"*

- **Chemical Sciences and Engineering Division Postdoctoral Seminar**, 2009, Argonne National Laboratory, Argonne IL. *"Electronic structure calculations with the graphically contracted function configuration interaction method"*
- **Argonne National Laboratory Postdoctoral Symposium**, 2008, Argonne National Laboratory, Argonne IL. *"Electronic structure calculations with graphically contracted functions"*

CONTRIBUTED TALKS

- **248th National Meeting of the American Chemical Society**, 2014, San Francisco, CA. "*Wave function analysis with Shavitt graph density in the graphically contracted function method*"
- **41st Midwest Theoretical Chemistry Conference**, 2009, Southern Illinois University, Carbondale, Carbondale, IL. "*Evaluation of determinant expansion coefficients and spin density matrices within the graphically contracted function method"*
- **40th Midwest Theoretical Chemistry Conference**, 2008, University of Michigan, Ann Arbor MI. *"Electronic structure calculations with graphically contracted functions"*
- **63rd International Molecular Spectroscopy Symposium**, 2008, Ohio State University, Columbus OH. *"CASSCF calculations via variational two-electron reduced-density matrix theory"*

POSTER PRESENTATIONS

- **42nd Midwest Theoretical Chemistry Conference**, 2010, Purdue University, West-Lafayett, IN. G. Gidofalvi and R. Shepard *"New developments and applications within the graphically contracted function configuration interaction method"*
- **50th Sanibel Symposium,** 2010, St. Simons Island, GA. G. Gidofalvi and R. Shepard. *"Excited-state calculations within the graphically contracted function method"*
- **49th Sanibel Symposium**, 2009, St. Simons Island, GA. G. Gidofalvi and R. Shepard. *"Evaluation of determinant expansion coefficients and spin density matrices within the graphically contracted function method"*
- **American Conference on Theoretical Chemistry**, 2008, Northwestern University, Evanston IL. G. Gidofalvi and R. Shepard. *"Electronic structure calculations with graphically contracted functions"*
- **229th National Meeting of the American Chemical Society**, 2005, San Diego CA. G. Gidofalvi and D. A. Mazziotti. *"Application of variational reduced-density-matrix theory to organic molecules"*

TEACHING EXPERIENCE

Gonzaga University

General Chemistry (CHEM 101), General Chemistry Lab (CHEM 101L), Inorganic Chemistry (CHEM 206), Inorganic Chemistry Lab (CHEM 206L), Quantitative Analysis Lab (CHEM 310L), Physical Chemistry I (CHEM 320), and Physical Chemistry II (CHEM 321)

University of Chicago

General Chemistry – Graduate Teaching Assistant — 2002-2003 and 2010
Physical Chemistry – Graduate Teaching Assistant — 2003

San Diego State University

General Chemistry – Undergraduate Teaching Assistant — 2000-2002

SERVICE

Coll./Univ.	Center For Undergraduate Research and Inquiry advisory committee	Fall 2016 - present
	GU Core – Scientific Inquiry sub-committee	Fall 2016 - present
	Academic Council Assessment Committee	Fall 2013 – present
	Co-director of the Intel Corporation Computational Science Laboratory	Spring 2012 – present
	Undergraduate Research Center Task Force	Fall 2015 – Spring 2016
Department:	Chemistry Department Program Promotion Committee	Fall 2015 – present
	Chemistry Biochemistry Curriculum Committee	Spring 2014 – present
	NTT Faculty Reappointment Committee	Fall 2013 – present
	Chemistry Department Assessment Committee	Spring 2011 – present
	Science Club Advisor	Fall 2012 – Spring 2017
	General Chemistry Textbook Committee	Spring 2013 and Spring 2015
	Coordinated Chemistry's GEL Weekend Course	2012 – 2016
	NTT Search Committee	Spring 2012
	General Chemistry Curriculum Review Committee	2012

Profession: Special session co-organizer: *"Strong Electron Correlation and Nonadiabatic Dynamics"*, 253rd National Meeting of the American Chemical Society

Article reviewer: Journal of Chemical Physics, Scientific Reports, Chemical Science, Journal of Physical Chemistry, Journal of Chemical Theory and Computation

Textbook reviewer: Gilbert's Chemistry: An Atom-Focused Approach, 1st edition; Chapters 16 – 18

TEACHING AND ADVISING RELATED WORKSHOPS ATTENDED

Assessment Institute — 2015
Indianapolis, IN

CCCE Computational Chemistry for Chemistry Educators workshop — 2013
Linfield College, OR

CTA Advising academy — 2011F – 2012S
Gonzaga University

cCWCS Computational and Theoretical Chemistry workshop — 2011
Westminster College, UT

cCWCS Renewable Energy workshop — 2010
Beloit College. WI

PROFESSIONAL MEMBERSHIPS

American Chemical Society: Member

ORAL PRESENTATIONS CO-AUTHORED WITH UNDERGRADUATE STUDENTS

- **Spokane Intercollegiate Research Conference**, April, 2014. Gonzaga University. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **Spokane Intercollegiate Research Conference**, April, 2014. Gonzaga University. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **22nd Annual M.J. Murdock Conference**, November, 2013. Lewis and Clark College. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **Spokane Intercollegiate Research Conference,** April, 2013. Whitworth University. Jake Zaragoza and Gergely Gidofalvi. *"The application of fractional Brownian motion to an ensemble average model"*
- **Spokane Intercollegiate Research Conference,** April, 2013. Whitworth University. Jake Zaragoza and Gergely Gidofalvi. *"The application of fractional Brownian motion to an ensemble average model"*
- **Spokane Intercollegiate Research Conference,** April, 2013. Whitworth University. Christopher Hastings and Gergely Gidofalvi. *"Natural orbitals for multiple electronic states"*

POSTER PRESENTATIONS CO-AUTHORED WITH UNDERGRADUATE STUDENTS

- **25th Annual M.J. Murdock Conference**, November, 2016. Gonzaga University. Matthew Gschiel and Gergely Gidofalvi. *"Improving the Efficiency and Accuracy of Molecular Modeling Through the use of Natural Orbitals"*
- **12th Annual Gonzaga Science Research Program Poster Session.** October, 2015. Gonzaga University. Truong-Son Nguyen and Gergely Gidofalvi.*"Modelling static correlation in large molecular systems: MCSCF calculations using 2-RDMs"*
- **12th Annual Gonzaga Science Research Program Poster Session.** October, 2015. Gonzaga University. Jack Gallagher and Gergely Gidofalvi. *"Assessing the accuracy of natural orbitals truncation schemes using electronic molecular properties"*
- **National Conference on Undergraduate Research,** April, 2015, Eastern Washington University. David Rodriguez-Perez and Gergely Gidofalvi. *"A complimentary tool for the visualization of molecular electronic structure"*
- **22nd Annual M.J. Murdock Conference,** November, 2014, Pacific University. David Rodriguez-Perez and Gergely Gidofalvi. *"A complimentary tool for the visualization of molecular electronic structure"*
- **11th Annual Gonzaga Science Research Program Poster Session.** October, 2014. Gonzaga

University. Alyssa Ylescupidez and Gergely Gidofalvi. *"Assessing the utility of natural orbitals in computational thermochemistry"*

- **National Conference on Undergraduate Research,** April, 2014. University of Kentucky. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **22nd Annual M.J. Murdock Conference**, November, 2013. Lewis and Clark College. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **10th Annual Gonzaga Science Research Program Poster Session**, October, 2013. Gonzaga University. Evan Jahrman and Gergely Gidofalvi. *"The use of natural orbitals in predicting molecular properties"*
- **21st Annual M.J. Murdock Conference**, October, 2012. Whitman College. Erinleigh Caughron, Christopher Hastings, and Gergely Gidofalvi. *"Efficient selection of orbitals for computing global potential energy surfaces"*
- **9th Annual Gonzaga Science Research Program Poster Session**, October, 2012. Gonzaga University. Erinleigh Caughron, Christopher Hastings, and Gergely Gidofalvi. *"Efficient selection of orbitals for computing global potential energy surfaces"*
- **20th Annual M.J. Murdock Conference**, November, 2011. Seattle University. Duncan Patton and Gergely Gidofalvi. *"A sum-over-states approach towards computing nonlinear optical properties of small molecules"*
- **8th Annual Gonzaga Science Research Program Poster Session,** October, 2011. Gonzaga University. John Gats and Gergely Gidofalvi. *"A complimentary approach for visualizing the electronic structure of molecules"*
- **8th Annual Gonzaga Science Research Program Poster Session,** October, 2011. Gonzaga University. Duncan Patton and Gergely Gidofalvi.*"A sum-over-states approach towards computing nonlinear optical properties of small molecules"*