

Curriculum Vitae

Richard Dawes

Missouri University of Science and Technology
120 Schrenk Hall, Department of Chemistry
400 West 11th Street
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Professional Preparation

| | | |
|----------------------|----------------|---|
| Post Doctoral Fellow | 2009-2010 | Sandia National Labs, Combustion Research Facility, Theoretical Molecular Dynamics, (Dr. Ahren W. Jasper) |
| NSERC PDF | 2006-2008 | University of Missouri-Columbia, Theoretical Molecular Dynamics, (Dr. Donald L. Thompson) |
| Post Doctoral Fellow | 2005-2006 | Université de Montréal, Theoretical Spectroscopy and Molecular Dynamics, (Dr. Tucker Carrington Jr.) |
| Ph. D. | 1999-2004 | University of Manitoba, Experimental and Theoretical Spectroscopy, (Dr. Kathleen M. Gough) |
| B.Sc. (Hons) | completed 1999 | University of Manitoba, Chemistry |

Appointments

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|---------------------|--------------|--|
| Assistant Professor | 2010-2014 | Missouri University of Science and Technology, Rolla, MO |
| Associate Professor | 2014-2018 | Missouri University of Science and Technology, Rolla, MO |
| Professor | 2018-present | Missouri University of Science and Technology, Rolla, MO |

Grants and Fellowships

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|-----------|--|-----------|
| 2019-2022 | DOE-Basic Energy Science | \$473,797 |
| 2016-2020 | NSF-Chemical Theory, Models and Computation | \$459,849 |
| 2013-2018 | DOE-Office of science early career award | \$750,000 |
| 2013-2016 | NSF-Chemical Theory, Models and Computation | \$433,843 |
| 2011-2012 | Missouri Research Board- <i>an accurate PES for ozone</i> | \$25,000 |
| 2006-2008 | Natural Sciences and Engineering Research Council of Canada (NSERC) Post-Doctoral Fellow | \$80,000 |

Professional Activities

- Co-Chair, Dynamics of Molecular Collisions meeting, Big Sky Montana, July 7-12, 2019, https://tofu.msu.montana.edu/cs/dmc_xxvii_2019
- Organizer of special symposium at ACS National meeting in Boston, August, 2018.
- 2017-2020 Faculty senate executive (current Parliamentarian).
- Director of campus High-Performance Computing Center (HPCC), <http://hpc.mst.edu/>
- Elected to three-year term on board of editors of *Journal of Molecular Spectroscopy* (Elsevier).
- Member of board of directors and organizer of “*International workshop on ozone and related atmospheric species*”, Reims France, Oct 4-6, 2017.
- Organizer of Telluride workshop: *New challenges for theory in chemical dynamics*, Jan 15-19, 2018.
- Flygare award lecture, *International Symposium on Molecular Spectroscopy*, June 22-26, 2015, Champaign-Urbana, Illinois.
- Organizer and session chair of focus session at APS National Meeting, *Nonadiabatic Dynamics*:

New Insights from Experiment and Theory, (San Antonio, TX, March 2-6, 2015).

-Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 7-11, 2014).

-Session chair at *International Symposium on Molecular Spectroscopy*, 69th meeting-June 16-20, 2014, Urbana-Champaign, Illinois.

-Session chair and invited speaker at Telluride workshop on *New Challenges for Theory in Chemical Dynamics* (Telluride, CO, January 12-17, 2014).

-Treasurer, local section (South Central Missouri) of American Chemical Society, 2013-2016

-Chair, local section (South Central Missouri) of American Chemical Society, 2012-2013

-Session chair (opening talk) at Dynamics of Molecular Collisions conference, session on *Atmosphere, Astrochemistry and Combustion* (Granlibakken NV, July 7-12, 2013).

-Session chair and invited speaker at annual meeting of the Canadian Society for Chemistry (CSC), *theory symposium* (May 26-30 2013, Quebec City, QC, Canada).

-Session chair and discussion leader at Gordon Conference on Molecular Energy Transfer, *non-adiabatic effects in energy transfer* (January 13-18, 2013, Ventura Beach Marriott).

-Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 9-13, 2012).

-Served on seven NSF review panels 2011-2018, with four in-person panels (Washington DC), and a 2018 site review.

-DOE panellist and site reviewer.

-Reviewer for numerous journals, e.g. *J. Chem. Phys.*, *J. Phys. Chem A*, *J. Mol. Spec.*, *Mol. Phys.*, *Chem. Phys. Lett.*, *J. Phys. Chem. Lett.*, *Nature Chem.*

Professional Societies

American Chemical Society (local section chair: 2012, treasurer: 2013-2016)

American Physical Society

Faculty Awards

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|------|---|--------|
| 2013 | Wilbur Tappmeyer Excellence in Teaching Award | \$1000 |
| 2013 | Missouri S&T Faculty Research Award | \$1000 |
| 2014 | Missouri S&T (Department) Excellence in Teaching Award | |
| 2014 | President's Award for <i>Early Career Excellence</i> (Missouri 4-Campus System) | \$5000 |
| 2015 | Missouri S&T Faculty Excellence Award | \$3000 |
| 2016 | Missouri S&T (Department) Excellence in Teaching Award | \$200 |
| 2016 | Missouri S&T (Department) Excellence in Service Award | \$333 |
| 2017 | Missouri S&T (Department) Excellence in Teaching Award | \$200 |
| 2017 | Missouri S&T (Department) Excellence in Service Award | \$333 |
| 2018 | Missouri S&T Faculty Excellence Award | \$3000 |
| 2018 | Missouri S&T (Department) Excellence in Teaching Award | \$200 |

Book Chapters

R. Dawes, E. L. Quintas-Sánchez. The Construction of Ab Initio-Based Potential Energy Surfaces. *Rev. Comput. Chem.* 2018, **31**:199-264. Reviews in Computational Chemistry, ed. K. B. Lipkowitz (Wiley-VCH, 2018)

The Quantum Theory of Atoms in Molecules, ed. R. Boyd and C. Matta (Wiley-VCH, 2007)

K.M. Gough, R. Dawes and J. Dwyer - QTAIM analysis of Raman scattering intensities: Insights into the relationship between molecular structure and electronic charge flow.

Peer-reviewed articles since (Sept 2010) arrival at Missouri S&T

- 1) S. Sur, E. Quintas Sánchez, S. A. Ndengué and R. Dawes, Development of a potential energy surface for the O₃–Ar system: rovibrational states of the complex, PCCP (advance article, DOI: 10.1039/C9CP01044K)
- 2) Ulrich Jentschura, Chandra Adhikari, Richard Dawes, Arthur Matveev, Nikolai Kolachevsky, Pressure Shifts in High-Precision Hydrogen Spectroscopy. I. Long-Range Atom-Atom and Atom-Molecule Interactions, *Journal of Physics B: Atomic, Molecular and Optical Physics*, 2019.
- 3) Shanyu Han, Xianfeng Zheng, Steve Ndengué, Yu Song, Richard Dawes, Daiqian Xie, Jingsong Zhang, Hua Guo, Dynamical interference in the vibronic bond breaking reaction of HCO, *Science Advances*, **5**, 2019 (DOI: 10.1126/sciadv.aau0582).
- 4) Steve A Ndengué, Yohann Scribano, David M Benoit, Fabien Gatti, Richard Dawes, Intermolecular rovibrational bound states of H₂OH₂ dimer from a MultiConfiguration Time Dependent Hartree approach, *Chemical Physics Letters*, **715**, (2019).
- 5) E Quintas-Sánchez, R Dawes, AUTOSURF: A Freely Available Program To Construct Potential Energy Surfaces, *Journal of Chemical Information and Modeling* **59** (1), 262-271 (2018).
- 6) R. Dawes and E. Quintas-Sánchez, The Construction Of Ab Initio-Based Potential Energy Surfaces, *Rev. Comput. Chem* **31**, 199-264 (2018).
- 7) M McCarthy, S Ndengué, R Dawes, The rotational spectrum and potential energy surface of the Ar–SiO complex, *The Journal of Chemical Physics* **149**, 134308 (2018).
- 8) S. Ndengue, R. Dawes, F. Gatti, H. Guo, The influence of Renner-Teller coupling between electronic states on inelastic scattering, *J. Phys. Chem. A*, **122**, 6381 (2018).
- 9) AJ Barclay, ARW McKellar, N Moazzen-Ahmadi, Richard Dawes, Xiao-Gang Wang, Tucker Carrington Jr, Infrared spectrum and intermolecular potential energy surface of the CO-O₂ dimer, *Physical Chemistry Chemical Physics*, **20**, 14431 (2018).
- 10) Hubert Cybulski, Christian Henriksen, Richard Dawes, Xiao-Gang Wang, Neha Bora, Gustavo Avila, Tucker Carrington, Berta Fernández, Ab initio study of the CO-N₂ complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum, *Physical Chemistry Chemical Physics*, **20**, 12624, 2018.
- 11) Kyle M Walker, Francois Lique, Richard Dawes, Fine and hyperfine collisional excitation of C₆H by He, *Monthly Notices of the Royal Astronomical Society* **473**, 1407, 2018.
- 12) Silver Nyambo, Brandon Uhler, Lloyd Muzangwa, Maxim Ivanov, Bradley K Welch, Richard Dawes, Scott A Reid, Reactive Pathways in the bromobenzene-ammonia dimer cation radical: evidence for a roaming halogen radical, *J. Mol. Struct.*, 1172, **113** (2018).
- 13) Andrew Powell, N.S. Dattani, RFK Spada, FBC Machado, H. Lischka, R. Dawes, Investigation of the ozone formation pathway: Comparisons of FCIQMC and fixed node DMC with icMRCI and ucMRCI. *J. Chem. Phys.* **147**, 094306 (2017).
- 14) Meng Huang, Terry A. Miller, Neal Kline and Richard Dawes, Studies via Near-IR Cavity Ringdown Spectroscopy and Electronic Structure Calculations of the Products of the Photolysis of Dihalomethane/N₂/O₂ Mixtures. *J. Phys. Chem. A* **121**, 98 (2017).
- 15) Steve Ndengué, Richard Dawes, Fabien Gatti and Hans-Dieter Meyer, Atom-triatom inelastic scattering with the MultiConfigurational Time Dependent Hartree approach, *Chem. Phys. Lett.* **668**, 42 (2017).
- 16) Kyle M. Walker, Francois Lique, Fabien Dumouchel and Richard Dawes, Inelastic rate coefficients for collisions of C₆H⁺ with H₂ and He. *Monthly Notices of the Royal Astronomical Society*, DOI: 10.1093/mnras/stw3065
- 17) Andrew D. Powell and Richard Dawes, Calculating potential energy curves with fixed-node diffusion Monte Carlo: CO and N₂, *J. Chem. Phys.* **145**, 224308 (2016).

- 18) Jun Li, Richard Dawes and Hua Guo, An accurate multi-channel multi-reference full-dimensional global potential energy surface for the lowest triplet state of H_2O_2 , *Phys. Chem. Chem. Phys.* **18**, 29825 (2016).
- 19) Xiao-gang Wang, Tucker Carrington Jr., and Richard Dawes, Computational study of the rovibrational spectra of $(\text{CO}_2)_2$, *J. Mol. Spec.* **330**, 179 (2016).
- 20) Kyle M. Walker, Fabien Dumouchel, Francois Lique, Richard Dawes, The first potential energy surfaces for the $\text{C}_6\text{H}-\text{H}_2$ and $\text{C}_6\text{H}-\text{He}$ collisional systems and their corresponding cross-sections. *J. Chem. Phys.* **145**, 024314 (2016).
- 21) Geoff Donoghue, Xiao-gang Wang, Richard Dawes and Tucker Carrington Jr., Computational study of the rovibrational spectra of $\text{CO}_2-\text{C}_2\text{H}_2$ and $\text{CO}_2-\text{C}_2\text{D}_2$. *J. Mol. Spec.* **330**, 170 (2016).
- 22) Steve Ndengué, Richard Dawes and Hua Guo, A new set of potential energy surfaces for HCO: Influence of Renner-Teller coupling on the bound and resonance vibrational states. *J. Chem. Phys.* **144**, 244301 (2016).
- 23) Richard Dawes and Steve Ndengué, Single- and multireference electronic structure calculations for constructing potential energy surfaces, *Int. Rev. Phys. Chem.* **35**, 441, (2016).
- 24) Steve Ndengue, Richard Dawes, Xiaogang Wang, Tucker Carrington Jr., Zhigang Sun and Hua Guo, Calculated vibrational states of ozone up to dissociation, *J. Chem. Phys.* **144**, 074302 (2016).
- 25) Moumita Majumder, Steve Ndengue, Richard Dawes, review (with author profile): automated construction of potential energy surfaces, *Molecular Physics* **114**, 1 (2016).
- 26) Phalgun Lolur, Richard Dawes, Michael Heaven, Theoretical study of vibronic perturbations in Magnesium Carbide, *Molecular Physics* **114**, 162 (2016).
- 27) Hua-Gen Yu, Steve Ndengue, Jun Li, Richard Dawes, Hua Guo, Vibrational levels of the simplest Criegee intermediate (CH_2OO) from full-dimensional Lanczos, MCTDH and MULTIMODE calculations, *J. Chem. Phys.* **143**, 084311 (2015).
- 28) Steve A. Ndengue, Richard Dawes, Fabien Gatti, Hans-Dieter Meyer, Resonances of HCO computed using an approach based on the multiconfigurational time-dependent Hartree method, *J. Phys. Chem. A* **119**, 12043 (2015).
- 29) Silver Nyambo, Cyrus Karshenas, Scott A. Reid, Phalgun Lolur, Richard Dawes, Towards a global model of spin-orbit coupling in the halocarbenes, *J. Chem. Phys.* **142**, 214304 (2015).
- 30) Zhigang Sun, Dequan Yu, Wenbo Xie, Jiayi Hou, Richard Dawes, Hua Guo, Kinetic isotope effect of the $^{16}\text{O} + ^{36}\text{O}_2$ and $^{18}\text{O} + ^{32}\text{O}_2$ isotope exchange reactions: Dominant role of reactive resonances revealed by an accurate time-dependent quantum wavepacket study, *J. Chem. Phys.* **142**, 174312 (2015).
- 31) Steve A. Ndengue, Richard Dawes and Fabien Gatti, Rotational Excitations in CO-CO Collisions at Low Temperature: Time Independent and Multiconfigurational Time Dependent Hartree Calculations, *J. Phys. Chem. A* **119**, 7712 (2015).
- 32) Jun Li, Bin Jiang, Hongwei Song, Jianyi Ma, Bin Zhao, Richard Dawes and Hua Guo, From ab initio Potential Energy Surfaces to State Resolved Reactivities: The $\text{X} + \text{H}_2\text{O} \leftrightarrow \text{HX} + \text{OH}$ ($\text{X}=\text{F}$, Cl , and $\text{O}(3\text{P})$) Reactions. *J. Phys. Chem. A* **119**, 4667 (2015).
- 33) Wenbo Xie, Lan Liu, Zhigang Sun, Hua Guo, Richard Dawes, State-to-state reaction dynamics of $^{18}\text{O} + ^{32}\text{O}_2$ studied by a time-dependent wavepacket method, *J. Chem. Phys.* **142**, 064308 (2015).
- 34) Moumita Majumder, Samuel E. Hegger, Richard Dawes, Sergei Manzhos, Xiao-Gang Wang, Tucker Carrington Jr., Jun Li, and Hua Guo, Explicitly-correlated MRCI-F12 potential energy surfaces for methane fit with several permutation invariant schemes and full-dimensional vibrational calculations, *Molecular Physics*, **113**, 1823, (2015).
- 35) Richard Dawes, Bin Jiang and Hua Guo, UV absorption spectrum and photodissociation channels of the simplest Criegee intermediate (CH_2OO), *J. Amer. Chem. Soc.* **137**, 50 (2015).

- 36) Sergei Manzhos, Richard Dawes and Tucker Carrington Jr., Neural Network-based Approaches for Building High Dimensional and Quantum Dynamics-Friendly Potential Energy Surfaces, *Int. J. Quantum Chemistry*, **115**, 1012, (2015).
- 37) Yaqin Li, Zhigang Sun, Bin Jiang, Daiqian Xie, Richard Dawes, Hua Guo, Rigorous Quantum Dynamics of O+O₂ exchange reactions on an ab initio potential energy surface substantiate the negative temperature dependence of rate coefficients, *J. Chem. Phys.* **141**, 081102 (2014).
- 38) Jun Li, Stuart Carter, Joel M. Bowman, Richard Dawes, Daiqian Xie, Hua Guo, High-Level, First-Principles, Full-Dimensional Quantum Calculation of the Ro-vibrational Spectrum of the Simplest Criegee Intermediate (CH₂OO), *J. Phys. Chem. Lett.* **5**, 2364 (2014).
- 39) Phalgun Lolur, Richard Dawes, 3D Printing of Molecular Potential Energy Surface Models, *J. Chem. Ed.* **91**, 1181 (2014).
- 40) Albert F. Wagner, Richard Dawes, Robert E. Continetti, Hua Guo, Theoretical/Experimental Comparison of Deep Tunneling Decay of Quasi-Bound H(D)OCO to H(D)+CO₂, *J. Chem. Phys.* **141**, 054304 (2014).
- 41) Aimable Kalume, Lisa George, Andrew D. Powell, Richard Dawes and Scott A. Reid, "Photoinduced electron transfer in donor-acceptor complexes of ethylene with molecular and atomic iodine", *J. Phys. Chem. A* **118**, 6838 (2014).
- 42) James Brown, Xiao-Gang Wang, Tucker Carrington, G.S. Grubbs II, Richard Dawes, Computational study of the rovibrational spectrum of CO₂-CS₂, *J. Chem. Phys.* **140**, 114303 (2014).
- 43) Jigar K. Mistry, Richard Dawes, Amitava Choudhury, Michael R. Van De Mark, 5-Mercapto-1,3,4-thiadiazole-2(3H)-thione: Synthesis and Structure of Alkylated Derivatives, *J. Het. Chem.* **51**, 747 (2014).
- 44) Richard Dawes, Phalgun Lolur, Anyang Li, Bin Jiang and Hua Guo, An accurate global potential energy surface for the ground state of ozone, *J. Chem. Phys.* **139**, 201103 (2013).
- 45) Thangavel Arumagum, Ian Elder, Chariklia Sotiriou-Leventis, Richard Dawes and Nicholas Leventis, Breaking aggregation and driving the keto-to-gem-diol Equilibrium of the N,N'-Dimethyl-2,6-diaza-9,10-anthraquinonediium dication to the keto Form by intercalation in cucurbit[7]uril, *J. Org. Chem.* **78**, 8297 (2013).
- 46) Thanh Lam Nguyen, Jun Li, Richard Dawes, John F. Stanton and Hua Guo, Accurate determination of barrier height and kinetics for the F + H₂O → HF + OH reaction, *J. Phys. Chem. A* **117**, 8864 (2013).
- 47) Ahren W. Jasper and Richard Dawes, Non-Born-Oppenheimer molecular dynamics of the spin-forbidden reaction O(³P) + CO(X ¹Σ⁺) ~> CO₂(X ¹Σ_g⁺), *J. Chem. Phys.* **139**, 154313 (2013).
- 48) Jun Li, Richard Dawes and Hua Guo, Kinetic and dynamic studies of the Cl(²P_u) + H₂O(X¹A₁) → HCl(X¹Σ⁺) + OH(X²Π) reaction on an ab initio based full-dimensional global potential energy surface of the ground electronic state of ClH₂O, *J. Chem. Phys.* **139**, 074302 (2013).
- 49) Jamin W. Perry, Richard Dawes, Albert F. Wagner and Donald L. Thompson, A classical trajectory study of the intramolecular dynamics and unimolecular dissociation of HO₂, *J. Chem. Phys.* **139**, 084319 (2013).
- 50) Richard Dawes, Xiao-Gang Wang and Tucker Carrington Jr., The CO dimer: a new potential energy surface and rovibrational calculations, *J. Phys. Chem. A*, **117**, 7612 (2013).
- 51) Beau J. Barker, Ivan O. Antonov, Jeremy M. Merritt, Vladimir E. Bondybey, Michael C. Heaven, Richard Dawes, Experimental and theoretical studies of the electronic transitions of BeC, *J. Chem. Phys.* **137**, 214313 (2012).
- 52) Chong Tao, Craig Richmond, Calvin Mukarakate, Scott H. Kable, George B. Baesckay, Eric C. Brown, Richard Dawes, Phalgun Lolur and Scott A. Reid, Spectroscopy and dynamics of the

- predissociated, quasi-linear S_2 state of chlorocarbene, *J. Chem. Phys.* **137**, 104307 (2012).
- 53) Jun Li, Richard Dawes and Hua Guo, An *ab initio* based full-dimensional global potential energy surface for $\text{FH}_2\text{O}(X^2A')$ and dynamics for the $\text{F} + \text{H}_2\text{O} \rightarrow \text{HF} + \text{HO}$ reaction, *J. Chem. Phys.* **137**, 094304 (2012).
 - 54) Jianyi Ma, Hua Guo and Richard Dawes, Low temperature rate constants for the $\text{N} + \text{CN} \rightarrow \text{N}_2 + \text{C}$ reaction: two-dimensional quantum capture calculations on an accurate potential energy surface, *Phys. Chem. Chem. Phys.* **14**(35) 12090-12093 (2012).
 - 55) Jun Li, Changjian Xie, Jianyi Ma, Yimin Wang, Richard Dawes, Daiqian Xie, Joel M. Bowman and Hua Guo, Quasi-classical trajectory study of the $\text{HO} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ reaction on a new *ab initio* based potential energy surface, *J. Phys. Chem. A* **116**, 5057-5067 (2012).
 - 56) James Brown, Xiao-Gang Wang, Richard Dawes, Tucker Carrington Jr, Computational study of the rovibrational spectrum of $(\text{OCS})_2$, *J. Chem. Phys.* **136**, 134306 (2012).
 - 57) Thangavel Arumagum, Chariklia Sotiriou-Leventis, Richard Dawes, Nicholas Leventis, Orientation of Pyrylium Guests in Cucurbituril Hosts, *J. Org. Chem.* **77**, 2263 (2012).
 - 58) Jun Li, Yimin Wang, Bin Jiang, Jianyi Ma, Richard Dawes, Daiqian Xie, Joel M. Bowman and Hua Guo, A chemically accurate potential energy surface for the $\text{HO} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ reaction, *J. Chem. Phys.* **136**, 041103 (2012).
 - 59) Richard Dawes, Phalgun Lolur, Jianyi Ma and Hua Guo, Highly Accurate Ozone Formation Potential and Implications for Kinetics, *J. Chem. Phys.* **135**, 081102 (2011).
 - 60) Raghu Sivaramakrishnan, Joe V. Michael, Albert. F. Wagner, Richard Dawes, Ahren W. Jasper, Lawrence. B. Harding, Yuri Georgievskii and Stephen J. Klippenstein, Roaming radicals in the thermal decomposition of dimethyl ether: Experiment and theory, *Combustion and Flame*, **158** 618 (2011).
 - 61) Chong Tao, Craig Richmond, Calvin Mukarakate, Richard Dawes, Scott H. Kable and Scott A. Reid, Optical-optical double resonance spectroscopy of the S_2 state of CHF and CDF: 1. Spectroscopy Analysis, *J. Chem. Phys.* **135**, 104315 (2011).
 - 62) Craig Richmond, Chong Tao, Calvin Mukarakate, Eric C. Brown, Richard Dawes, Scott H. Kable and Scott A. Reid, Optical-optical double resonance spectroscopy of the S_2 state of CHF and CDF: 2. Predissociation and mode-specific dynamics, *J. Chem. Phys.* **135**, 104316 (2011).
 - 63) Richard Dawes, Jason R. Dwyer, Weixing Qu, and Kathleen M. Gough, QTAIM investigation of the electronic structure and large Raman scattering intensity of bicyclo-[1.1.1]-pentane, *J. Phys. Chem A* **115**, 13149 (2011).
 - 64) Xiao-Gang Wang, Tucker Carrington Jr., Richard Dawes and Ahren W. Jasper, The vibration-rotation-tunneling spectrum of the polar and T-shaped-N-in isomers of $(\text{NNO})_2$, *J. Mol. Spec.* **268**, 53 (2011).
 - 65) Ali Siavosh-Haghighi, Richard Dawes, Thomas D. Sewell, Donald L. Thompson, A Molecular Dynamics Study of Classical Vibrational Spectra in Hydrostatically Compressed Crystalline Nitromethane, *J. Phys. Chem. B*, **114**, 17177 (2010).
 - 66) Richard Dawes, Xiao-Gang Wang, Ahren W. Jasper, Tucker Carrington Jr., Nitrous oxide dimer: A new potential energy surface and ro-vibrational spectrum of the polar isomer, *J. Chem. Phys.* **133**, 134304 (2010).
 - 67) Andrew J. Binder, Richard Dawes, Ahren W. Jasper, Jon P. Camden, The role of excited electronic states in hypervelocity collisions: Enhancement of the $\text{O}(^3\text{P}) + \text{HCl} \rightarrow \text{OCl} + \text{H}$ reaction channel, *J. Phys. Chem. Lett.* **1**, 2940, (2010).

Invited and contributed talks since (Sept 2010) arrival at Missouri S&T

Upcoming

- 1) Marquette University, Chemistry Dept. Seminar, May 3, 2019.
- 2) International Symposium on Molecular Spectroscopy, Champaign-Urbana, IL, June 17-21, 2019.
- 3) Dynamics of Molecular Collisions meeting, Big Sky Montana, July 7-12, 2019. Speaker and Co-organizer.

Given

* Indicates regional recruiting and outreach

- 1) Telluride Symposium – Intermolecular Interactions, Telluride CO, March 17-22, 2019.
- 2) Visiting professor – two week lecture series, Le Havre, France, Oct 10-24, 2018.
- 3) ACS Boston 2018 - Organizing special symposium - From Potential Energy Surfaces to Dynamics and Kinetics, Boston, MA, August 19-23, 2018.
- 4) Telluride Symposium - Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride CO, July 17-21, 2018.
- 5) International Symposium on Molecular Spectroscopy, Champaign-Urbana, IL, June 18-22, 2018.
- *6) Invited seminar at Mizzou, MO, May 1, 2018.
- 7) Telluride workshop - Hydrides: from Earth to Space. Telluride, CO, March 19-22, 2018.
- *8) Invited seminar at College of the Ozarks, MO, Feb 28, 2018.
- 9) Organizer of Telluride Workshop: New Challenges for Theory in Chemical Dynamics, Telluride, CO, Jan 15-19, 2018.
- 10) Int. workshop on ozone and related atmospheric species, Reims France, Oct 4-6, 2017.
- *11) Invited seminar at Truman University, MO, Aug 24, 2017.
- 12) Atlantic Theoretical Chemistry Symposium, Aug 1, 2017, Halifax, NS, Canada.
- 13) Automated construction of PESs for Intermolecular Interactions, TSRC Workshop, Picos de Europa, Spain, 07/09/2017.
- 14) Theoretical Studies of Spectroscopy and Dynamics, (Le Havre, France, Mar 23, 2017).
- 15) Theoretical Studies of Spectroscopy and Dynamics, (Paris-Saclay, Mar 20, 2017).
- 16) Calculations of spectroscopy and scattering dynamics using interpolated ab initio potentials, Invited talk, TACC2016, Aug 28-Sept 2, 2016, Seattle, WA, USA.
- 17) Calculations of spectroscopy and scattering dynamics using interpolated ab initio potentials, Invited talk, ISTCP IX, July 17-22, 2016 Grand Forks, ND, USA.
- 18) Calculated vibrational states of ozone up to dissociation, talk at *International Symposium on Molecular Spectroscopy*, June 20-24, 2016, Champaign-Urbana, Illinois.
- 19) Theoretical studies of spectroscopy and dynamics using interpolated potential energy surfaces. Department seminar, University of Louisville, February 26, 2016.
- 20) 63rd Pacific Conference on Spectroscopy and Dynamics, Invited talk, Asilomar, CA, January 29, 2016.
- 21) New challenges for theory in chemical dynamics. Invited talk, Telluride workshop, Telluride CO, January 13 2016.
- 22) New insights from quantum dynamics and ab initio potentials in high dimensional systems. Invited talk, Pacificchem, December 16 2015.
- 23) Electronic structure and potential fitting methods suitable for multistate reactive surfaces, Invited talk, iCOMET symposium, Chengdu, China, October 12, 2015
- 24) Flygare award lecture, *International Symposium on Molecular Spectroscopy*, June 22-26, 2015, Champaign-Urbana, Illinois.
- 25) Electronic structure and potential fitting methods suitable for multistate reactive surfaces, Invited talk, DICP symposium, Dalian, China, June 4, 2015
- 26) Construction of Potential Energy Surfaces for Excited Electronic States, Invited talk, National

- ACS meeting, Denver, CO, March 22-26, 2015.
- 27) Construction of Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Saint Louis University, St Louis, MO, March 20.
 - 28) Electronic Structure and Potential Fitting Methods Suitable for Multistate Reactive Surfaces, Invited talk, National APS meeting, San Antonio, TX, March 2, 2015
 - 29) Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Université Montpellier, France, November 24, 2014.
 - 30) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Université de Reims, Reims, France, November 18, 2014.
 - 31) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Midwestern Regional ACS, Columbia, MO, November 13, 2014.
 - 32) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Argonne National Labs, August 20, 2014.
 - 33) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 7-11, 2014).
 - 34) Session chair (opening talk) International Symposium on Molecular Spectroscopy, 69th meeting- June 16-20, 2014 Urbana-Champaign, Illinois.
 - 35) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, University of New Mexico, February 28, 2014.
 - 36) Session chair and invited speaker at Telluride workshop on *New Challenges for Theory in Chemical Dynamics* (Telluride, CO, January 12-17, 2014).
 - 37) Invited talk at 2nd International Workshop “Spectroscopy and dynamics of ozone and related species”, Reims, France, October 2-4, 2013.
 - 38) Session chair (opening talk) at Dynamics of Molecular Collisions conference, session on *Atmosphere, Astrochemistry and Combustion* (Granlibakken NV, July 7-12, 2013).
 - 39) Session chair and invited speaker at annual meeting of the Canadian Society for Chemistry (CSC), *theory symposium* (May 26-30 2013, Quebec City, QC, Canada).
 - 40) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, UC-Merced, (Feb 22, 2013).
 - 41) Session chair and discussion leader at Gordon Research Conference on *Molecular energy transfer*, January 13-18, 2013, Ventura beach Marriott).
 - 42) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, invited talk, Queen’s University, Canada, (Jan 10, 2013).
 - 43) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 9-13, 2012).
 - 44) “High-accuracy potentials for vdWs systems”, 67th International Symposium on Molecular Spectroscopy, Columbus OH (06/21/2012).
 - 45) “Molecular Potential Energy Surfaces for Spectroscopy and Dynamics: Numerical Methods for Accurate Multidimensional Interpolation”, MICAMS seminar, Department of Mathematics, Missouri University of Science and Technology, 02/27/2012.
 - 46) “Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics”, Dynamite Seminar, University of Missouri-Columbia, 02/21/2012.
 - 47) “Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics”, Telluride Workshop, 01/02/2012.
 - 48) “Theoretical molecular dynamics”, Department Seminar- Emory University, 10/03/2011.
 - 49) “Construction of Potential Energy Surfaces for Spectroscopy and Dynamics”, Department

Seminar, Missouri State University, 09/07/2011.
50) “Construction of Potential Energy Surfaces for Spectroscopy and Dynamics”, Quantum Reactive Scattering 11, Santa Fe NM, 07/20/2011.
4851) “Dynamically weighted MRCI: ozone”, Dynamics of Molecular Collisions, Snowbird UT, 07/13/2011.

Thesis Advisement

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|---------------|---|
| Phalgun Lolur | Ph.D. Graduate (successful October 2015 thesis defence) |
| Andrew Powell | Ph.D. Candidate (Successful June 2017 thesis defence) |
| Bradley Welch | Ph.D. Candidate (Scheduled June 2019 thesis defence) |
| Sangeeta Sur | Ph.D. Student |

Postdoctoral Mentoring

Steve Ndengué (current DOE project)
Ernesto Quintas Sánchez (current NSF project)
Moumita Majumder (previous, now faculty member at Indian Institute of Technology Dharwad)