Curriculum Vitae

Richard Dawes

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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

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	2018-2021	Missouri University of Science and Technology, Rolla, MO
Adjunct Professor	2021-2024	Missouri University of Science and Technology, Rolla, MO
Program Officer	2019-2020	National Science Foundation, Alexandria, VA
Program Lead	2020-present	National Science Foundation, Alexandria, VA

Grants and Fellowships

2024-2027	DOE-Basic Energy Science	$493,103
2019-2022	NSF-MRI (withdrew as lead PI due to NSF employment)	$2,800,000
2019-2023	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-*an accurate PES for ozone*	$25,000
2006-2008	Natural Sciences and Engineering Research Council of Canada (NSERC) Post-Doctoral Fellow	$80,000

Professional Activities

-Chair, Dynamics of Molecular Collisions meeting, Snowbird, Utah, July 2023.
-American Physical Society, Division Chemical Physics, executive (member-at-large), 2022
-Co-Chair, Dynamics of Molecular Collisions meeting, Big Sky Montana, July, 2019.
-Organizer of special symposium at ACS National meeting in Boston, August, 2018.
-2017-2020 Faculty senate executive (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 (recent member-at-large Division of Chemical Physics)

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

1) Bostan, Dulat, Bikramaditya Mandal, Carolin Joy, Michał Żółtowski, François Lique, Jérôme Loreau, Ernesto Quintas-Sánchez, Adrian Batista-Planas, Richard Dawes, and Dmitri Babikov.

"Mixed quantum/classical calculations of rotationally inelastic scattering in the CO+ CO system: a comparison with fully quantum results." *Physical Chemistry Chemical Physics* 26, no. 8 (2024): 6627-6637.
2) Tela, Hervé Tajouo, Ernesto Quintas-Sánchez, Marie-Lise Dubernet, Yohann Scribano, Richard Dawes, Fabien Gatti, and Steve Ndengué. "Rovibrational states calculations of the H 2 O–HCN heterodimer with the multiconfiguration time dependent Hartree method." *Physical Chemistry Chemical Physics* 25, no. 46 (2023): 31813-31824.
3) Dumouchel, Fabien, Ernesto Quintas-Sánchez, Christian Balança, Richard Dawes, François Lique, and Nicole Feautrier. "Collisional excitation of C2H− by H2: New interaction potential and scattering calculations." *The Journal of Chemical Physics* 158, no. 16 (2023).
4) Ndengué, Steve, Ernesto Quintas-Sánchez, Richard Dawes, Christopher C. Blackstone, and David L. Osborn. "Temperature dependence of the electronic absorption spectrum of NO2." *The Journal of Physical Chemistry A* 127, no. 29 (2023): 6051-6062.
5) Olejnik, Artur, Hubert Jóźwiak, Maciej Gancewski, Ernesto Quintas-Sánchez, Richard Dawes, and Piotr Wcisło. "Ab initio quantum scattering calculations and a new potential energy surface for the HCl (X1Σ+)–O2 (X3Σg−) system: Collision-induced line shape parameters for O2-perturbed R (0) 0–0 line in H35Cl." *The Journal of Chemical Physics* 159, no. 13 (2023).
6) Sun, Ge, Shanyu Han, Xianfeng Zheng, Yu Song, Yuan Qin, Richard Dawes, Daiqian Xie, Jingsong Zhang, and Hua Guo. "Unimolecular dissociation dynamics of electronically excited HCO (Ã 2 A′): rotational control of nonadiabatic decay." *Faraday Discussions* 238 (2022): 236-248.
7) Ajili, Yosra, Ernesto Quintas-Sánchez, Bilel Mehnen, Piotr S. Żuchowski, Filip Brzęk, Nayla El-Kork, Marko Gacesa, Richard Dawes, and Majdi Hochlaf. "Theoretical study of the CO 2–O 2 van der Waals complex: potential energy surface and applications." *Physical Chemistry Chemical Physics* 24, no. 47 (2022): 28984-28993.
8) Dzenis, Karlis, Alexandre Faure, B. A. McGuire, A. J. Remijan, P. J. Dagdigian, C. Rist, Richard Dawes, Ernesto Quintas-Sánchez, François Lique, and M. Hochlaf. "Collisional Excitation and Non-LTE Modeling of Interstellar Chiral Propylene Oxide." *The Astrophysical Journal* 926, no. 1 (2022): 3.
9) Denis-Alpizar, Otoniel, Ernesto Quintas-Sánchez, and Richard Dawes. "State-to-state rate coefficients for HCS+ in rotationally inelastic collisions with H2 at low temperatures." *Monthly Notices of the Royal Astronomical Society* 512, no. 4 (2022): 5546-5551.
10) Zadrożny, Adam, Hubert Jóźwiak, Ernesto Quintas-Sánchez, Richard Dawes, and Piotr Wcisło. "Ab initio quantum scattering calculations for the CO–O2 system and a new CO–O2 potential energy surface: O2 and air broadening of the R (0) line in CO." *The Journal of Chemical Physics* 157, no. 17 (2022).
6)
11) Ndengué, Steve, Ernesto Quintas-Sánchez, Richard Dawes, and David Osborn. "The low-lying electronic states of NO2: Potential energy and dipole surfaces, bound states, and electronic absorption spectrum." *The Journal of Physical Chemistry A* 125, no. 25 (2021): 5519-5533.
12) Han, Shanyu, Ge Sun, Xianfeng Zheng, Yu Song, Richard Dawes, Daiqian Xie, Jingsong Zhang, and Hua Guo. "Rotational modulation of Ã 2 A ″-state photodissociation of HCO via Renner–Teller nonadiabatic transitions." *The Journal of Physical Chemistry Letters* 12, no. 28 (2021): 6582-6588.
13) Gancewski, Maciej, Hubert Jóźwiak, Ernesto Quintas-Sánchez, Richard Dawes, Franck Thibault, and Piotr Wcisło. "Fully quantum calculations of O2–N2 scattering using a new potential energy surface: Collisional perturbations of the oxygen 118 GHz fine structure line." *The Journal of chemical physics* 155, no. 12 (2021).

14) Balança, Christian, Ernesto Quintas-Sánchez, Richard Dawes, Fabien Dumouchel, François Lique, and Nicole Feautrier. "Inelastic rate coefficients for collisions of C4H− with H2." *Monthly Notices of the Royal Astronomical Society* 508, no. 1 (2021): 1148-1155.
15) Quintas-Sánchez, Ernesto, Richard Dawes, and Otoniel Denis-Alpizar. "Theoretical study of the HCS+–H2 van der Waals complex: potential energy surface, rovibrational bound states, and rotationally inelastic collisional cross sections." *Molecular Physics* 119, no. 21-22 (2021): e1980234.
16) Bop, Cheikh T., François Lique, Alexandre Faure, Ernesto Quintas-Sánchez, and Richard Dawes. "Non-LTE modelling of cyanoacetylene: evidence for isomer-specific excitation." Monthly Notices of the Royal Astronomical Society 501, no. 2 (2021): 1911-1919.
17) Quintas-Sánchez, Ernesto, and Richard Dawes. "Spectroscopy and scattering studies using interpolated ab initio potentials." *Annual Review of Physical Chemistry* 72, no. 1 (2021): 399-421.
18) Desrousseaux, Benjamin, Ernesto Quintas-Sánchez, Richard Dawes, Sarantos Marinakis, and François Lique. "Collisional excitation of interstellar PN by H_2: New interaction potential and scattering calculations." The Journal of Chemical Physics 154, no. 3 (2021): 034304.
19) Bop, Cheikh Tidiane, Ernesto Quintas-Sánchez, Sangeeta Sur, Mathurin Robin, François Lique, and Richard Dawes. "Inelastic scattering in isotopologues of O_2–Ar: the effects of mass, symmetry, and density of states." Physical Chemistry Chemical Physics (2021).
20) Desrousseaux, Benjamin, François Lique, Javier R. Goicoechea, Ernesto Quintas-Sánchez, and Richard Dawes. "CF+ excitation in the interstellar medium." Astronomy & Astrophysics 645 (2021): A8.
21) Endres, Eric S., Steve Ndengué, Olga Lakhmanskaya, Seunghyun Lee, Francesco A. Gianturco, Richard Dawes, and Roland Wester. "Temperature-dependent rotationally inelastic collisions of OH− and He." *Physical Review A* 103, no. 5 (2021): 052807.
22) Han, Shanyu, Carolyn E. Gunthardt, Richard Dawes, Daiqian Xie, Simon W. North, and Hua Guo. "Origin of the “odd” behavior in the ultraviolet photochemistry of ozone." Proceedings of the National Academy of Sciences 117, no. 35 (2020): 21065-21069.
23) Quintas-Sánchez, Ernesto, Richard Dawes, Kelvin Lee, and Michael C. McCarthy. "Automated Construction of Potential Energy Surfaces Suitable to Describe van der Waals Complexes with Highly Excited Nascent Molecules: The Rotational Spectra of Ar–CS (v) and Ar–SiS (v)." The Journal of Physical Chemistry A 124, no. 22 (2020): 4445-4454.
24) Yang, Dongzheng, Junxiang Zuo, Jing Huang, Xixi Hu, Richard Dawes, Daiqian Xie, and Hua Guo. "A global full-dimensional potential energy surface for the K2Rb2 complex and its lifetime." The journal of physical chemistry letters 11, no. 7 (2020): 2605-2610.
25) Ben Khalifa, M., E. Quintas-Sánchez, R. Dawes, K. Hammami, and L. Wiesenfeld. "Rotational quenching of an interstellar gas thermometer: CH3CN-He collisions." Physical Chemistry Chemical Physics 22, no. 31 (2020): 17494-17502.
26) Quintas-Sánchez, Ernesto, Richard Dawes, Xiao-Gang Wang, and Tucker Carrington. "Computational study of the rovibrational spectrum of CO 2–N 2." Physical Chemistry Chemical Physics 22, no. 39 (2020): 22674-22683.
27) Sur, Sangeeta, Steve A. Ndengué, Ernesto Quintas-Sánchez, Cheikh Bop, François Lique, and Richard Dawes. "Rotationally inelastic scattering of O 3–Ar: state-to-state rates with the multiconfigurational time dependent Hartree method." Physical Chemistry Chemical Physics 22, no. 4 (2020): 1869-1880.
28) Ndengué, Steve, Yohann Scribano, Fabien Gatti, and Richard Dawes. "State-to-state inelastic rotational cross sections in five-atom systems with the multiconfiguration time dependent Hartree method." The Journal of chemical physics 151, no. 13 (2019): 134301.

29) Castro-Juárez, Eduardo, Xiao-Gang Wang, Tucker Carrington Jr, Ernesto Quintas-Sánchez, and Richard Dawes. "Computational study of the ro-vibrational spectrum of CO–CO2." The Journal of chemical physics 151, no. 8 (2019): 084307.
30) Desrousseaux, Benjamin, Ernesto Quintas-Sánchez, Richard Dawes, and François Lique. "Collisional Excitation of CF+ by H2: Potential Energy Surface and Rotational Cross Sections." The Journal of Physical Chemistry A 123, no. 45 (2019): 9637-9643.
31) Welch, Bradley K., Richard Dawes, David H. Bross, and Branko Ruscic. "An automated thermochemistry protocol based on explicitly correlated coupled-cluster theory: The methyl and ethyl peroxy families." The Journal of Physical Chemistry A 123, no. 26 (2019): 5673-5682.
32) Bop, Cheikh T., Fidel A. Batista-Romero, Alexandre Faure, Ernesto Quintas-Sánchez, Richard Dawes, and François Lique. "Isomerism effects in the collisional excitation of cyanoacetylene by molecular hydrogen." ACS Earth and Space Chemistry 3, no. 7 (2019): 1151-1157.
33) Hu, Xixi, Junxiang Zuo, Changjian Xie, Richard Dawes, Hua Guo, and Daiqian Xie. "An ab initio based full-dimensional potential energy surface for OH+ O 2⇄ HO 3 and low-lying vibrational levels of HO 3." Physical Chemistry Chemical Physics 21, no. 25 (2019): 13766-13775.
34) Faure, Alexandre, Paul J. Dagdigian, Claire Rist, Richard Dawes, Ernesto Quintas-Sánchez, François Lique, and Majdi Hochlaf. "Interaction of chiral propylene oxide (CH3CHCH2O) with helium: potential energy surface and scattering calculations." ACS Earth and Space Chemistry 3, no. 6 (2019): 964-972.
35) Sur, Sangeeta, Ernesto Quintas-Sánchez, Steve A. Ndengué, and Richard Dawes. "Development of a potential energy surface for the O 3–Ar system: rovibrational states of the complex." Physical Chemistry Chemical Physics 21, no. 18 (2019): 9168-9180.
36) 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.
37) 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).
38) Steve A Ndengué, Yohann Scribano, David M Benoit, Fabien Gatti, Richard Dawes, Intermolecular rovibrational bound states of H_2OH_2 dimer from a MultiConfiguration Time Dependent Hartree approach, *Chemical Physics Letters*, **715**, (2019).
39) 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).
40) R. Dawes and E. Quintas-Sánchez, The Construction Of Ab Initio-Based Potential Energy Surfaces, *Rev. Comput. Chem* **31**, 199-264 (2018).
41) 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).
42) 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).
43) 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-O_2 dimer, Physical Chemistry Chemical Physics, **20**, 14431 (2018).
44) Hubert Cybulski, Christian Henriksen, Richard Dawes, Xiao-Gang Wang, Neha Bora, Gustavo Avila, Tucker Carrington, Berta Fernández, Ab initio study of the CO-N_2 complex: a new highly accurate intermolecular potential energy surface and rovibrational spectrum, Physical Chemistry

Chemical Physics, **20**, 12624, 2018.
45) 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.
46) 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).
47) 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).
48) 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/N_2/O_2 Mixtures. *J. Phys. Chem. A* **121**, 98 (2017).
49) 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).
50) Kyle M. Walker, Francois Lique, Fabien Dumouchel and Richard Dawes, Inelastic rate coefficients for collisions of C_6H^- with H_2 and He. *Monthly Notices of the Royal Astronomical Society*, **DOI**: 10.1093/mnras/stw3065
51) Andrew D. Powell and Richard Dawes, Calculating potential energy curves with fixed-node diffusion Monte Carlo: CO and N_2, *J. Chem. Phys.* **145**, 224308 (2016).
52) 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).
53) Xiao-gang Wang, Tucker Carrington Jr., and Richard Dawes, Computational study of the rovibrational spectra of $(CO_2)_2$ *J. Mol. Spec.* **330**, 179 (2016).
54) Kyle M. Walker, Fabien Dumouchel, Francois Lique, Richard Dawes, The first potential energy surfaces for the $C6H^-$-H_2 and $C6H^-$-He collisional systems and their corresponding cross-sections. *J. Chem. Phys.* **145**, 024314 (2016).
55) Geoff Donoghue, Xiao-gang Wang, Richard Dawes and Tucker Carrington Jr., Computational study of the rovibrational spectra of CO_2-C_2H_2 and CO_2-C_2D_2. *J. Mol. Spec.* **330**, 170 (2016).
56) 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).
57) Richard Dawes and Steve Ndengué, Single- and multireference electronic structure calculations for constructing potential energy surfaces, *Int. Rev. Phys. Chem.* **35**, 441, (2016).
58) 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).
59) Moumita Majumder, Steve Ndengue, Richard Dawes, review (with author profile): automated construction of potential energy surfaces, *Molecular Physics* **114**, 1 (2016).
60) Phalgun Lolur, Richard Dawes, Michael Heaven, Theoretical study of vibronic perturbations in Magnesium Carbide, *Molecular Physics* **114**, 162 (2016).
61) 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).
62) 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).
63) 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).
64) Zhigang Sun, Dequan Yu, Wenbo Xie, Jiayi Hou, Richard Dawes, Hua Guo, Kinetic isotope effect of the $^{16}O + {}^{36}O_2$ and $^{18}O + {}^{32}O_2$ isotope exchange reactions: Dominant role of reactive resonances revealed by an accurate time-dependent quantum wavepacket study, *J. Chem. Phys.* **142**, 174312 (2015).
65) 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).
66) 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 X + H2O ↔ HX + OH (X=F, Cl, and O(3P)) Reactions. *J. Phys. Chem. A* **119**, 4667 (2015).
67) Wenbo Xie, Lan Liu, Zhigang Sun, Hua Guo, Richard Dawes, State-to-state reaction dynamics of $^{18}O + {}^{32}O_2$ studied by a time-dependent wavepacket method, *J. Chem. Phys.* **142**, 064308 (2015).
68) 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).
69) 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).
70) 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).
71) Yaqin Li, Zhigang Sun, Bin Jiang, Daiqian Xie, Richard Dawes, Hua Guo, Rigorous Quantum Dynamics of $O+O_2$ exchange reactions on an ab initio potential energy surface substantiate the negative temperature dependence of rate coefficients, *J. Chem. Phys.* **141**, 081102 (2014).
72) 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 (CH_2OO), *J. Phys. Chem. Lett.* **5**, 2364 (2014).
73) Phalgun Lolur, Richard Dawes, 3D Printing of Molecular Potential Energy Surface Models, *J. Chem. Ed.* **91**, 1181 (2014).
74) Albert F. Wagner, Richard Dawes, Robert E. Continetti, Hua Guo, Theoretical/Experimental Comparison of Deep Tunneling Decay of Quasi-Bound H(D)OCO to $H(D)+CO_2$, *J. Chem. Phys.* **141**, 054304 (2014).
75) 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).
76) James Brown, Xiao-Gang Wang, Tucker Carrington, G.S. Grubbs II, Richard Dawes, Computational study of the rovibrational spectrum of CO_2-CS_2, *J. Chem. Phys.* **140**, 114303 (2014).
77) 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).
78) 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).

79) 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).
80) Thanh Lam Nguyen, Jun Li, Richard Dawes, John F. Stanton and Hua Guo, Accurate determination of barrier height and kinetics for the F + H_2O → HF + OH reaction, *J. Phys. Chem. A* **117**, 8864 (2013).
81) Ahren W. Jasper and Richard Dawes, Non-Born-Oppenheimer molecular dynamics of the spin-forbidden reaction $O(^3P)$ + $CO(X\ ^1\Sigma^+)$ ~> $CO_2(X\ ^1\Sigma_g^+)$, *J. Chem. Phys.* **139**, 154313 (2013).
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83) Jamin W. Perry, Richard Dawes, Albert F. Wagner and Donald L. Thompson, A classical trajectory study of the intramolecular dynamics and unimolecular dissociation of HO_2, *J. Chem. Phys.* **139**, 084319 (2013).
84) 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).
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Invited and contributed talks since (Sept 2010) arrival at Missouri S&T

1) MolSSI workshop on rovibrational spectroscopy, Nov 14-15, 2019.
2) Marquette University, Chemistry Dept. Seminar, May 3, 2019.
3) International Symposium on Molecular Spectroscopy, Champaign-Urbana, IL, June 17-21, 2019.
4) Dynamics of Molecular Collisions meeting, Big Sky Montana, July 7-12, 2019. Speaker and Co-organizer.
5) Telluride Symposium – Intermolecular Interactions, Telluride CO, March 17-22, 2019.
6) Visiting professor – two week lecture series, Le Havre, France, Oct 10-24, 2018.
7) ACS Boston 2018 - Organizing special symposium - From Potential Energy Surfaces to Dynamics and Kinetics, Boston, MA, August 19-23, 2018.
8) Telluride Symposium - Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride CO, July 17-21, 2018.
9) International Symposium on Molecular Spectroscopy, Champaign-Urbana, IL, June 18-22, 2018.
6) Invited seminar at Mizzou, MO, May 1, 2018.
10) Telluride workshop - Hydrides: from Earth to Space. Telluride, CO, March 19-22, 2018.
11) Invited seminar at College of the Ozarks, MO, Feb 28, 2018.
12) Organizer of Telluride Workshop: New Challenges for Theory in Chemical Dynamics, Telluride, CO, Jan 15-19, 2018.
13) Int. workshop on ozone and related atmospheric species, Reims France, Oct 4-6, 2017.
14) Invited seminar at Truman University, MO, Aug 24, 2017.

15) Atlantic Theoretical Chemistry Symposium, Aug 1, 2017, Halifax, NS, Canada.
16) Automated construction of PESs for Intermolecular Interactions, TSRC Workshop, Picos de Europa, Spain, 07/09/2017.
17) Theoretical Studies of Spectroscopy and Dynamics, (Le Havre, France, Mar 23, 2017).
18) Theoretical Studies of Spectroscopy and Dynamics, (Paris-Saclay, Mar 20, 2017).
19) Calculations of spectroscopy and scattering dynamics using interpolated ab initio potentials, Invited talk, TACC2016, Aug 28-Sept 2, 2016, Seattle, WA, USA.
20) Calculations of spectroscopy and scattering dynamics using interpolated ab initio potentials, Invited talk, ISTCP IX, July 17-22, 2016 Grand Forks, ND, USA.
21) Calculated vibrational states of ozone up to dissociation, talk at *International Symposium on Molecular Spectroscopy*, June 20-24, 2016, Champaign-Urbana, Illinois.
22) Theoretical studies of spectroscopy and dynamics using interpolated potential energy surfaces. Department seminar, University of Louisville, February 26, 2016.
23) 63rd Pacific Conference on Spectroscopy and Dynamics, Invited talk, Asilomar, CA, January 29, 2016.
24) New challenges for theory in chemical dynamics. Invited talk, Telluride workshop, Telluride CO, January 13 2016.
25) New insights from quantum dynamics and ab initio potentials in high dimensional systems. Invited talk, Pacifichem, December 16 2015.
26) Electronic structure and potential fitting methods suitable for multistate reactive surfaces, Invited talk, iCOMET symposium, Chengdu, China, October 12, 2015
27) Flygare award lecture, *International Symposium on Molecular Spectroscopy*, June 22-26, 2015, Champaign-Urbana, Illinois.
28) Electronic structure and potential fitting methods suitable for multistate reactive surfaces, Invited talk, DICP symposium, Dalian, China, June 4, 2015
29) Construction of Potential Energy Surfaces for Excited Electronic States, Invited talk, National ACS meeting, Denver, CO, March 22-26, 2015.
30) Construction of Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Saint Louis University, St Louis, MO, March 20.
31) Electronic Structure and Potential Fitting Methods Suitable for Multistate Reactive Surfaces, Invited talk, National APS meeting, San Antonio, TX, March 2, 2015
32) Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Université Montpellier, France, November 24, 2014.
33) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Université de Reims, Reims, France, November 18, 2014.
34) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Midwestern Regional ACS, Columbia, MO, November 13, 2014.
35) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Argonne National Labs, August 20, 2014.
36) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 7-11, 2014).
37) Session chair (opening talk) International Symposium on Molecular Spectroscopy, 69th meeting- June 16-20, 2014 Urbana-Champaign, Illinois.
38) Automated Construction of ab initio Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, University of New Mexico, February 28, 2014.
39) Session chair and invited speaker at Telluride workshop on *New Challenges for Theory in*

Chemical Dynamics (Telluride, CO, January 12-17, 2014).
40) Invited talk at 2nd International Workshop "Spectroscopy and dynamics of ozone and related species", Reims, France, October 2-4, 2013.
41) Session chair (opening talk) at Dynamics of Molecular Collisions conference, session on *Atmosphere, Astrochemistry and Combustion* (Granlibakken NV, July 7-12, 2013).
42) 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).
43) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, UC-Merced, (Feb 22, 2013).
44) Session chair and discussion leader at Gordon Research Conference on *Molecular energy transfer*, January 13-18, 2013, Ventura beach Marriott).
45) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, invited talk, Queen's University, Canada, (Jan 10, 2013).
46) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 9-13, 2012).
47) "High-accuracy potentials for vdWs systems", 67th International Symposium on Molecular Spectroscopy, Columbus OH (06/21/2012).
48) "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.
49) "Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics", Dynamite Seminar, University of Missouri-Columbia, 02/21/2012.
50) "Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics", Telluride Workshop, 01/02/2012.
51) "Theoretical molecular dynamics", Department Seminar- Emory University, 10/03/2011.
52) "Construction of Potential Energy Surfaces for Spectroscopy and Dynamics", Department Seminar, Missouri State University, 09/07/2011.
53) "Construction of Potential Energy Surfaces for Spectroscopy and Dynamics", Quantum Reactive Scattering 11, Santa Fe NM, 07/20/2011.
54) "Dynamically weighted MRCI: ozone", Dynamics of Molecular Collisions, Snowbird UT, 07/13/2011.

Thesis Advisement

Phalgun Lolur	Ph.D. Graduate (October 2015 thesis defence)
Andrew Powell	Ph.D. Graduate (June 2017 thesis defence)
Bradley Welch	Ph.D. Graduate (June 2019 thesis defence)
Sangeeta Sur	Ph.D. Graduate (June 2020 thesis defence)
Adrian Batista-Planas	Ph.D. Candidate (expected fall 2025 thesis defence)

Postdoctoral Mentoring

Steve Ndengué (previous, now faculty at Haverford)

Ernesto Quintas Sánchez (now research faculty on current DOE project)

Moumita Majumder (previous, now faculty member at Indian Institute of Technology Dharwad)