Curriculum Vitae

Richard Dawes

Missouri University of Science and Technology
120 Schrenk Hall, Department of Chemistry
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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.	1999-2005	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-present	Missouri University of Science and Technology, Rolla, MO

Grants and Fellowships

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

-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-present

-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 four NSF review panels 2011-2015, with three in-person panels (Washington DC).

-DOE reviewer of student scholarship awards as well as research proposals for the BES program.

-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.*

Professional Societies

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

American Physical Society

Faculty Awards

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 *Early Career Excellence* (Missouri 4-Campus System)	$5000

Book Chapter

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) Phalgun Lolur, Richard Dawes, Michael Heaven, Theoretical study of vibronic perturbations in Magnesium Carbide, *Molecular Physics* (in production: TMPH-2015-0396.R1)
2) 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).
3) 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* (Article ASAP, June 12, 2015, **DOI:** 10.1021/acs.jpca.5b04642).
4) 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).
5) 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).
6) 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).
7) 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).
8) 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).

9) 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).
10) 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).
11) 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).
12) 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).
13) 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).
14) Phalgun Lolur, Richard Dawes, 3D Printing of Molecular Potential Energy Surface Models, *J. Chem. Ed.* **91**, 1181 (2014).
15) 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).
16) 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).
17) 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).
18) Jigar K. Mistry, Richard Dawes, AmitavaChoudhury, 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).
19) 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).
20) 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).
21) Thanh Lam Nguyen, Jun Li, Richard Dawes, John F. Stanton and Hua Guo, Accurate determination of barrier height and kinetics for the $F + H_2O \rightarrow HF + OH$ reaction, *J. Phys. Chem. A* **117**, 8864 (2013).
22) Ahren W. Jasper and Richard Dawes, Non-Born-Oppenheimer molecular dynamics of the spin-forbidden reaction $O(^3P) + CO(X\ ^1\Sigma^+) \sim> CO_2(X\ ^1\Sigma_g^+)$, *J. Chem. Phys.* **139**, 154313 (2013).
23) Jun Li, Richard Dawes and Hua Guo, Kinetic and dynamic studies of the $Cl(^2P_u) + H_2O(X^1A_1) \rightarrow HCl(X^1\Sigma^+) + OH(X^2\Pi)$ reaction on an ab initio based full-dimensional global potential energy surface of the ground electronic state of ClH_2O, *J. Chem. Phys.* **139**, 074302 (2013).
24) 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).

25) 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).
26) 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)**.**
27) Chong Tao, Craig Richmond, Calvin Mukarakate, Scott H. Kable, George B. Bacskay, 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)**.**
28) Jun Li, Richard Dawes and Hua Guo, An *ab initio* based full-dimensional global potential energy surface for $FH_2O(X^2A')$ and dynamics for the $F + H_2O \rightarrow HF + HO$ reaction, *J. Chem. Phys.* **137**, 094304 (2012).
29) Jianyi Ma, Hua Guo and Richard Dawes, Low temperature rate constants for the $N + CN \rightarrow N_2 + C$ reaction: two-dimensional quantum capture calculations on an accurate potential energy surface, *Phys. Chem. Chem. Phys.* **14**(35) 12090-12093 (2012).
30) Jun Li, Changjian Xie, Jianyi Ma, Yimin Wang, Richard Dawes, Daiqian Xie, Joel M. Bowman and Hua Guo, Quasi-classical trajectory study of the $HO + CO \rightarrow H + CO_2$ reaction on a new ab initio based potential energy surface, *J. Phys. Chem.A* **116**, 5057-5067 (2012).
31) James Brown, Xiao-Gang Wang, Richard Dawes, Tucker Carrington Jr, Computational study of the rovibrational spectrum of $(OCS)_2$, *J. Chem. Phys.* **136**, 134306 (2012).
32) Thangavel Arumagum, Chariklia Sotiriou-Leventis, Richard Dawes, Nicholas Leventis, Orientation of Pyrylium Guests in Cucurbituril Hosts, *J. Org. Chem.* **77**, 2263 (2012).
33) 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 $HO + CO \rightarrow H + CO_2$ reaction, *J. Chem. Phys.* **136**, 041103 (2012).
34) Richard Dawes, Phalgun Lolur, Jianyi Ma and Hua Guo, Highly Accurate Ozone Formation Potential and Implications for Kinetics, *J. Chem. Phys.* **135**, 081102 (2011).
35) 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).
36) 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).
37) 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).
38) 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).
39) 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 $(NNO)_2$, *J. Mol. Spec.* **268**, 53 (2011).
40) 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).

41) 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).
42) Andrew J. Binder, Richard Dawes, Ahren W. Jasper, Jon P. Camden, The role of excited electronic states in hypervelocity collisions: Enhancement of the $O(^3P) + HCl \rightarrow OCl + H$ reaction channel, *J. Phys. Chem. Lett*. **1**, 2940, (2010).

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

1) Flygare award lecture, *International Symposium on Molecular Spectroscopy*, June 22-26, 2015, Champaign-Urbana, Illinois.
2) Electronic structure and potential fitting methods suitable for multistate reactive surfaces, Invited talk, DICP symposium, Dalian, China, June 4, 2015
3) Construction of Potential Energy Surfaces for Excited Electronic States, Invited talk, National ACS meeting, Denver, CO, March 22-26, 2015.
4) Construction of Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Saint Louis University, St Louis, MO, March 20.
5) Electronic Structure and Potential Fitting Methods Suitable for Multistate Reactive Surfaces, Invited talk, National APS meeting, San Antonio, TX, March 2, 2015
6) Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Université Montpellier, France, November 24, 2014.
7) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Université de Reims, Reims, France, November 18, 2014.
8) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Midwestern Regional ACS, Columbia, MO, November 13, 2014.
9) The Electronic Structure, Spectroscopy and Dynamics of Small Molecules, Invited talk, Argonne National Labs, August 20, 2014.
10) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on multiple potential energy surfaces* (Telluride, CO, July 7-11, 2014).
11) Session chair (opening talk) International Symposium on Molecular Spectroscopy, 69th meeting- June 16-20, 2014 Urbana-Champaign, Illinois.
12) Automated Construction of ab initio Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, University of New Mexico, February 28, 2014.
13) Session chair and invited speaker at Telluride workshop on *New Challenges for Theory in Chemical Dynamics* (Telluride, CO, January 12-17, 2014).
14) Invited talk at 2nd International Workshop "Spectroscopy and dynamics of ozone and related species", Reims, France, October 2-4, 2013.
15) Session chair (opening talk) at Dynamics of Molecular Collisions conference, session on *Atmosphere, Astrochemistry and Combustion* (Granlibakken NV, July 7-12, 2013).
16) 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).
17) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, UC-Merced, (Feb 22, 2013).
18) Session chair and discussion leader at Gordon Research Conference on *Molecular energy transfer*, January 13-18, 2013, Ventura beach Marriott).
19) Automated Construction of *ab initio* Potential Energy Surfaces for Spectroscopy and Dynamics, Invited talk, Queen's University, Canada, (Jan 10, 2013).
20) Session chair and invited speaker at Telluride workshop on *spectroscopy and dynamics on*

multiple potential energy surfaces (Telluride, CO, July 9-13, 2012).
21) "High-accuracy potentials for vdWs systems", 67th International Symposium on Molecular Spectroscopy, Columbus OH (06/21/2012).
22) "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.
23) "Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics", Dynamite Seminar, University of Missouri-Columbia, 02/21/2012.
24) "Dynamically-weighted multistate multi-reference configuration interaction (MRCI) calculations for spectroscopy and dynamics", Telluride Workshop, 01/02/2012.
25) "Theoretical molecular dynamics", Department Seminar- Emory University, 10/03/2011.
26) "Construction of Potential Energy Surfaces for Spectroscopy and Dynamics", Department Seminar, Missouri State University, 09/07/2011.
27) "Construction of Potential Energy Surfaces for Spectroscopy and Dynamics", Quantum Reactive Scattering 11, Santa Fe NM, 07/20/2011.
28) "Dynamically weighted MRCI: ozone", Dynamics of Molecular Collisions, Snowbird UT, 07/13/2011.

Teaching at Missouri S&T

SP 2011: Chem 455	2 students	4.00 teaching effectiveness
FS 2011: Chem 243	18 students	3.00 teaching effectiveness
SP 2012: Chem 241	52 students	2.94 teaching effectiveness
FS 2012: Chem 243	12 students	4.00 teaching effectiveness
SP 2013: Chem 344	11 students	3.89 teaching effectiveness
FS 2013: Chem 243	17 students	3.75 teaching effectiveness
SP 2014: Chem 401	6 students	3.50 teaching effectiveness
FS 2013: Chem 3430	16 students	3.60 teaching effectiveness
SP 2015: Chem 5430	5 students	3.67 teaching effectiveness

Wilbur Tappmeyer Excellence in undergraduate teaching award ($1000), 2012-2013
Department 300 level teaching award 2014

Committee Service at Missouri S&T

Graduate Students Admissions Committee	Departmental Committee	2011
Space Committee	Departmental Committee	2012
Personnel Committee	Departmental Committee	2012
Promotion and Tenure Committee	Departmental Committee	2012
IT Committee	Campus Committee	2012
Chair, Hiring Committee	Department Committee	2013
Department Strategic Planning Committee	Department Committee	2013
Chair, Research Computing IT-subcommittee	Campus Committee	2013
Chair, Graduate Recruitment Committee	Department Committee	2014-present
Personnel Committee	Departmental Committee	2014-present

Thesis Advisement

Phalgun Lolur	PhD Candidate (scheduled October 2015 thesis defence)
Andrew Powell	PhD Candidate
Bradley Welch	PhD Candidate
Sangeeta Sur	PhD Candidate

Postdoctoral Mentoring

Steve Ndengue

Moumita Majumder