JOSEPH S. FRANCISCO

EDUCATION

B.S.	University of Texas at Austin	1977
Ph.D.	Massachusetts Institute of Technology	1983

PROFESSIONAL EXPERIENCE

Research Fellow, Cambridge University,	1983-1985
Provost Postdoctoral Fellow, MIT	1985-1986
Assistant Professor, Wayne State University	1986-1990
Associate Professor, Wayne State University	1990-1994
Visiting Associate, California Institute of Technology	1991
Visiting Scientist, Jet Propulsion Laboratory, Caltech	1993
Professor, Purdue University	1995-2006
Sterling A. Brown Visiting Professor, Williams College	1998
Visiting Senior Fellow, Universita di Bologna, Italy	2003
William E. Moore Distinguished Professor, Purdue University	2006-present
Professeur Invité, Université de Paris-Est, France	2011
Visiting Professor, Uppsala Universitet, Sweden	2012
Associate Dean, College of Science, Purdue University	2010-2013
Honorary International Chair Professor, National Taipei University, Taiwan	2012-2015
David Parkin Visiting Professor, University of Bath, England	2013-2014

HONORS AND AWARDS

Presidential Young Investigator Award, National Science Foundation, 1988
Alfred P. Sloan Research Fellow, 1990
Camille and Henry Dreyfus Teacher-Scholar Award, 1990
Outstanding Teacher Award, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, 1992
John Simon Guggenheim Fellow, 1993
AAAS Mentor Award, American Association for the Advancement of Science, 1994
Percy L. Julian Award for Pure and Applied Research, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, 1995
Fellow, American Physical Society, 1998
University Faculty Scholar, Purdue University, 1999
Alexander von Humboldt Senior U.S. Scientist Award, 2001
Fellow, American Association for the Advancement of Science, 2001
Herbert Newby McCoy Award, Purdue University, 2007
Fellow, American Academy of Arts and Sciences, 2010
Edward W. Morley Medal, American Chemical Society Cleveland Section, 2011
Fellow, American Chemical Society, 2012
Member, National Academy of Sciences, 2013

DISTINGUISHED APPOINTMENTS

Naval Research Advisory Committee, Department of Navy, 1994-1996
Sigma Xi National Lecturer, 1995-1997
Army Research Science Board, Department of Army, 1997-1999
President, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, 2005-2007

President, American Chemical Society, 2010
President's Committee on the National Medal of Science, White House, 2010-2012, and 2013-2016
Alexander von Humboldt Foundation International Advisory Board, 2014-present

HONORARY DEGREE
Doctor of Science, *honoris causa*, Tuskegee University, 2010
Doctor of Science, *honoris causa*, University of Arkansas at Little Rock, 2011
Doctor of Science, *honoris causa*, Knox College, 2012
Doctor of Science, *honoris causa*, University of South Florida, 2012

PUBLICATIONS JOSEPH S. FRANCISCO

A. Scholarly books published:

. J.I. Steinfeld, J.S. Francisco and W.L. Hase, *Chemical Kinetics and Dynamics*, Prentice-Hall, Englewood Cliffs, NJ (January, 1989), pp. 1-548.
Japanese Translation: Prentice Hall, Japan (1995).
Second Edition: Prentice Hall, Englewood Cliffs, NJ (August, 1998).

B. Chapters published:

9. C.M. Rosedo-Reyes, M. Martinez-Aviles and J.S. Francisco, Computational Study of the Reaction of n-Bromopropane with OH Radicals and Cl atoms, "Applications of Theoretical Methods to Atmospheric Science", in Advances in Quantum Chemistry, M.E. Goodsite and M.S. Johnson, eds., Vol. 55, Chapter 11, Elsevier (2008) pp. 215-244.
8. S. Guha and J.S. Francisco, "Stratospheric Bromine Chemistry: Insights from Computational Studies," in *Computational Chemistry: Review of Current Trends*, J. Leszczynski, ed., World Scientific Publishing (Singapore) (1999) pp. 75-148.
7. J.S. Francisco and J.A. Montgomery, "Theoretical Studies of the Energetics of Radicals," in *Energetics of Organic Free Radicals*, J.A.M. Simoes, A. Greenberg, J.F. Liebman, eds., Vol. 4, Chapter 4, Blackie Academic & Professional Co., (1995) pp. 110-149.
6. Z. Li, T.S. Dibble and J.S. Francisco, "A Review of the Experimental and Theoretical Progress in Understanding the Role of CX_3 Radicals in Atmospheric Chemical Processes," in *Advances in Physical Chemistry*, C-Y. Ng, ed., World Publishing Co., Pte. Ltd. (1995) pp. 686-743.
5. S.P. Sander, R. Friedl and J.S. Francisco, "Progress in the Understanding of Inorganic Chlorine Compounds in Atmospheric Processes," in *Advances in Physical Chemistry*, C-Y. Ng, ed., World Publishing Co. Pte. Ltd. (1995) pp. 876-921.
4. J.S. Francisco and I.H. Williams, "Atmospheric Chemistry of Organic Halides," in *Chemistry of Functional Groups*, S. Patai and Z. Rappoport, eds., John Wiley and Sons (1995) pp. 1559-1583.
3. J.S. Francisco and M.M. Maricq, "Atmospheric Photo-oxidation Processes of Alternative Halocarbons," in *Advances in Photochemistry*, D. Volman and D. Neckers, eds., Vol. 20, John Wiley and Sons, (1995) pp. 79-163.
2. M.S. Gordon, J.S. Francisco and H.B. Schlegel, "Theoretical Investigation of the Thermochemistry and Thermal Decomposition of Silanes, Halosilanes, and Alkylsilanes," in *Advances in Silicon Chemistry*, G.C. Larson, ed., Vol. 2, JAI Press Inc. (1993) pp. 137-185.

1. J.S. Francisco and J.I. Steinfeld, "Photochemistry, Photophysics, and Spectroscopy of IR Multiple Photon Excitation" in *Advances in Multiphoton Processes and Spectroscopy*, S. H. Lin, ed., Vol. 3, Taylor and Francis (1986) pp. 79-175.

C. Journal articles published

Refereed journals: Total 460, those since 2005 listed below

460. S.B. Yaghlane, R. Linquerri, M. Hochlaf, C. E. Cotton, and J.S. Francisco, Ab Initio Structural and Spectroscopic Study of HPS^x and HSP^x (x=0,+1,-1) in the Gas Phase, *J. Chem. Phys.*, **139**, 174313 (2013).

459. J.M. Anglada, G.J. Hoffman, L.V. Slipchenko, M.Martins-Costa, M.F. Ruiz-Lopez, J.S. Francisco, The Atmospheric Significance of Water Clusters and Ozone-Water Complexes, *J. Phys. Chem. A.,* **117**, 10381-10396 (2013).

458. N. Lu, R.M. Ley, C.E. Cotton, J.S. Francisco and E. Negishi, Molecular Tuning of the C-H…F-C Hydrogen Bond, *J. Phys. Chem. A*, **117**, 8256-8262 (2013).

457. C.E. Cotton, J.S. Francisco, and W. Klemperer, Computational Study of the Linear Proton Bound Ion-Molecule Complexes of $HCNH^+$ with HCN and HNC, *J. Chem. Phys.*, **139**, 014304 (2013).

456. M.K. Hazra, J.S. Francisco and A. Sinha, Gas Phase Hydrolysis of Formaldehyde to Form Methanediol: Impact of Formic Acid Catalysis, *J. Phys. Chem. A.,* **117**, 11704-11710 (2013).

455. C. Love, L. Tan, J.S. Francisco and Y. Xia, Competition of Charge- vs. Radical-Directed Fragmentation of Gas-Phase Protonated Cysteine Sulfinyl Radicals, *J. Am. Chem. Soc*., **135**, 6226-6233 (2013).

454. O. Yazidi, A.B. Houria, J.S. Francisco, M. Hochlaf, Electronic States, Conical Intersections and Spin-Rovibronic Spectroscopy of the Nitrogen Oxide Sulfide Radical, *J. Chem. Phys*., **138**, 104318 (2013).

453. C.E. Cotton, J.S. Francisco, and A. P. Mitruschchenkov, Structural and Spectroscopic Study of the van der Waals Complex of PN with HNP^+, *J. Chem. Phys.*, **138**, 074314 (2013).

452. M.C. Green, D.G. Fedorov, K. Kitaura, J.S. Francisco, L.V. Slipchenko, Open-Shell Pair Interaction Energy Decomposition Analysis (PIEDA): Formulation and Application to Hydrogen Abstraction in Tripeptides, *J. Chem. Phys.*, **138**, 074111 (2013).

451. X. Huang , R.C. Fortenberry, Y. Wang, J.S. Francisco, T.D. Crawford, J.M. Bowman, and, T.J. Lee, Dipole Surfaces and Infrared Intensities for the cis- and trans-HOCO and DOCO Radicals, *J. Phys. Chem. A.*, **117**,6932-6939 (2013).

450. M.G. Delcey, R. Lindh, R. Linguerri, M. Hochlaf, J.S. Francisco, Structure and Spectroscopic Properties of the Hydroxymethyl Peroxy ($HOCH_2OO$) Radical, *J. Chem. Phys.,* **138**, 021105 (2013).

449. M.C. Green, S. Stelzleni, and J.S. Francisco, A Spectral Marker for C_α Damage in Beta Peptides, *J. Phys. Chem. A.,* **117**, 550-565 (2013).

448. M. Torrent-Sucarrat, J. S. Francisco, and J.M. Anglada, Sulfuric Acid as Auto-Catalyst in the Formation of Sulfuric Acid, *J. Am. Chem. Soc*., **134**, 20632-20644 (2012); see also *Science,* **339**,120 (2013).

447. M.T.C. Martins-Costa, J.M. Anglada, J.S. Francisco, and M.F. Ruiz-Lopez, Reactivity of Small Radicals of Atmospheric Interest at the Air/Water Interface, *Angew. Chem. Int. Ed.*, **51**, 5413-5417 (2012).

446. L. Vereecken and J.S. Francisco, Theoretical Studies of Atmospheric Reaction Mechanisms in the Troposphere, *Chem. Soc. Rev.*, **41**, 6259-6293 (2012).

445. M.T.C. Martins-Costa, J.M. Anglada, J.S. Francisco, and M.F. Ruiz-Lopez, Reactivity of Volatile Organic Compounds at the Surface of a Water Droplet, *J. Am. Chem. Soc*., **134**, 11821-11827 (2012).

444. R. Linquerri and J.S. Francisco, Structural and Spectroscopic Properties of the H_2O_2-H_2O Complex, *J. Chem. Phys.*, **137**, 214312 (2012).

443. R.C. Fortenberry, X. Huang, J.S. Francisco, T.D. Crawford, T.J. Lee, Fundamental Vibrational Frequencies and Spectroscopic Constants of $HOCS^+$ and $HSCO^+$, and Isotopologues via Quartic Force Fields *J. Phys. Chem. A.*, **116**, 9582-9590 (2012).

442. S.B. Yaghlane, J.S. Francisco, and M. Hochlaf, Accurate Theoretical Study of PS^q (where q=0, +1, -1) in the Gas Phase, *J. Chem. Phys.*, **136,** 244309 (2012).

441. M. Hochlaf, R. Linquerri, S.S. Dalal, and J.S. Francisco, Theoretical Study of the Spectroscopically Relevant Parameters for the Detection of HNP^q and HPN^q (q=0,+1,-1) in the Gas Phase, *J. Chem. Phys.*, **136**, 244311 (2012).

440. M.K. Hazra, J.S. Francisco, and A. Sinha, Computational Study of Hydrogen-Bonded Complexes of HOCO with Acids: $HOCO^{\cdots}HCOOH$, $HOCO^{\cdots}H_2SO_4$ and $HOCO^{\cdots}H_2CO_3$, *J. Chem. Phys.*, **137**, 064319 (2012).

439. C.E. Cotton, J.S. Francisco, R. Linquerri, and A. P. Mitruschchenkov, Structural and Spectroscopic Study of the van der Waals Complex of CO with HCO^+ and the Isoelectronic CS with HCS^+ Complex, *J. Chem. Phys.*, **136**, 184307 (2012).

438. X. Zeng, H. Beckers, H. Willner and J.S. Francisco, Experimental Observation of 16-Electron Molecules: SPN, SNP, and Cyclic PSN, *Angew. Chem. Int. Ed.*, **51**, 3334-3339 (2012).

437. R.J. Buszek, J. S. Francisco and J.R. Barker, Water Effect on the OH + HCl Reaction, *J. Phys. Chem. A.*, **116**, 4712-4719 (2012).

436. R.C. Fortenberry, X. Huang, J.S. Francisco, T.D. Crawford, T.J. Lee, Quartic Force Field Predictions of the Fundamental Vibrational Frequencies and Spectroscopic Constants of the Cations $HOCO^+$ and $DOCO^+$, *J. Chem. Phys*., **136**, 234309 (2012).

435. A.C. Davis and J.S. Francisco, Hydrogen Migrations in Alkylcycloalky Radicals: Implications for Chain Branching Reactions in Fuels, *Chem. Euro. J.,* **18**, 11296-11305 (2012).

434. R.J. Buszek, M. Torrent-Sucarrat, J.M. Anglada, and J.S. Francisco, The Effects of a Single Water on the OH + H_2O_2 Reaction, *J. Phys. Chem. A.*, **116**, 5821-5829 (2012).

433. S.I. Kokkila, P.P. Bera, J.S. Francisco, T.J. Lee, A Group Increment Scheme for Infrared Absorption Intensities of Greenhouse Gases, *J. Mol. Struct.*, **1009**, 89-95 (2012).

432. A.C. Davis and J.S. Francisco, Ab Initio Study of Chain Branching Reactions Involving Second Generation Products in Hydrocarbon Combustion Mechanisms, *Phys. Chem. Chem. Phys.*, **14**, 1343-1351 (2012).

431. A.C. Davis, and J. S. Francisco, Ab Initio Study of Key Branching Reactions in Biodiesel and Frischer-Tropsch Fuels, *J. Am. Chem. Soc.*, **133**,19110-19124 (2011).

430. J. Clark, J.C. Hansen, and J.S. Francisco, NH_x-Acid Complexes and Their Role in the Formation of Atmospheric Aerosols, *J. Chem. Phys.*, **135**, 244305 (2011).

429. C.C. Wu, H.C. Lin, Y.B. Chang, P.Y. Tsai, Y.Y. Yeh, R.C. Lin, and J.S. Francisco, Br_2 Molecular Elimination in Photolysis of $(COBr)_2$ at 248 nm by Using Cavity Ring-down Absorption Spectroscopy: A Photodissociation Channel Being Ignored, *J. Chem. Phys.*, **135**, 234308 (2011).

428. R.C. Fortenberry, X. Huang, J.S. Francisco, T.D. Crawford, T.J. Lee, Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields for *cis*-HOCO: the Radical and the Anion, *J. Chem. Phys.*, **135**, 214303 (2011).

427. R.J. Buszek, J.M. Anglada, and J.S. Francisco, Water Effect on Atmospheric Reactions, *Int. Rev. Phys. Chem.(Invited)*, **30**, 335-369 (2011).

426. A.C. Davis and J.S. Francisco, Reactivity Trends Within Alkoxy Radical Reactions Responsible for Chain Branching, *J. Am. Chem. Soc.*, **133**, 18208-18219 (2011).

425. R.C. Fortenberry, X. Huang, J.S. Francisco, T.D. Crawford, T.J. Lee, The *trans*-HOCO Radical: Quartic Force Fields, Vibrational Frequencies, and Spectroscopic Constants, *J. Chem. Phys.*, **135**, 134301 (2011).

424. D. J. Wuebbles, K.O. Patten, D. Wang, D. Youn, M. Martinez-Aviles, J. S. Francisco, Three-dimensional model evaluation of the Ozone Depletion Potentials for n-propyl bromide, trichloroethylene and perchloroethylene, *Atmos. Chem. Phys.*, **11**, 2371-2380 (2011).

423. S. Du, J.S. Francisco, and J.R. Lyons, Determination of the $S+S_2$ Rate Constant for Recombination by Quasi-Classical Trajectory Calculations, *J. Chem. Phys.*, **134**,154508 (2011).

422. A.C. Davis and J.S. Francisco, *Ab initio* Study of Hydrogen Migration Across Alkyl Radicals, *J. Phys. Chem. A.*, **115**, 2966-2977 (2011).

421. K.A. Peterson and J.S. Francisco, *Ab initio* Spectroscopic Characterization of the HNNO and ONHN Radicals, *J. Chem. Phys.*, **134**, 084308 (2011).

420. J. Gonzalez, J.M. Anglada, R.J. Buszek, and J.S. Francisco, The Impact of Water on the OH + HOCl Reaction, *J. Am. Chem. Soc.*, **133**, 3345-3353 (2011).

419. M. Torrent-Sucarrat, M.F. Ruiz-Lopez, M.Martins-Costa, J.S. Francisco, J.M. Anglada, Protonation of Water Clusters Induced by the Hydroperoxyl Radical Surface Absorption, *Chem. Euro. J.*, **17**, 5076-5085 (2011).

418. R.J. Buszek, A. Sinha, and J.S. Francisco, The Isomerization of Methoxy Radical: Intramolecular Hydrogen Atom Transfer Mediated Through Acid Catalysis, *J. Am. Chem. Soc.*, **133**, 2013-2015 (2011).

417. J.S. Francisco, J.T. Muckerman, and H.G. Yu, HOCO Radical Chemistry, *Acc. Chem. Res.*, **43**, 1519-1526 (2010).

416. A.C. Davis and J.S. Francisco, *Ab initio* Study of Hydrogen Migration Across Alkylperoxy Radicals, *J. Phys. Chem. A.*, **114**, 11492-11505 (2010).

415. C.J. Christiansen and J.S. Francisco, Atmospheric Oxidation of Trichloroethylene: An *Ab Initio* Study, *J. Phys. Chem. A.,* **114**, 9163-9176 (2010).

414. C.J. Christiansen and J.S. Francisco, Atmospheric Oxidation of Tetrachloroethylene: An *Ab Initio* Study, *J. Phys. Chem. A.*, **114**, 9177-9191 (2010).

413. P.P. Bera, J.S. Francisco, and T.J. Lee, Design Strategies to Minimize the Radiative Efficiency of Global Warming Molecules, *Proc. Natl. Acad. Sci. USA.*, **107**, 9049-9054 (2010).

412. H.Q. Doan, A. C. Davis, J.S. Francisco, Primary Steps in the Reaction of OH Radicals with Model Amides, *J. Phys. Chem. A.*, **113**, 5342-5357 (2010).

411. D.J. Grant, E.B. Garner III, M.H. Matus, M.T. Nguyen, K.A. Peterson, J.S. Francisco and D.A. Dixon, The Thermodynamic Properties of the XO_2, X_2O, XYO, X_2O_2, and XYO_2 (X,Y=Cl, Br, and I) Isomers, *J. Phys. Chem. A.*, **114**, 4254-4265 (2010).

410. C.J. Christiansen, S.S. Dalal, J.S. Francisco, A.M. Mebel, J.S. Gaffney, Hydroxyl Radical Substitution in Halogenated Carbonyls: Oxalic Acid Formation, *J. Phys. Chem. A.*, **114**, 2806-2820 (2010).

409. P. Soloveichik, B.A. O'Donnell, M.I. Lester, J.S. Francisco and A.B. McCoy, Infrared Spectrum and Stability of the OH-H_2O Complex: Experiment and Theory, *J. Phys. Chem. A.*, **114**, 1529-1538 (2010).

408. H.G. Yu and J.S. Francisco, Ab initio and RRKM Study of the Reaction of ClO with HOCO Radicals, *J. Phys. Chem. A.*, **113**, 12932-12941 (2009).

407. W. Eisfeld and J.S. Francisco, Structure, Spectroscopic Properties, and Photochemistry of the Hydroxymethoxy Radical, *J. Chem. Phys.*, **131**, 134313 (2009).

406. S. Du, J.S. Francisco, G.K. Schenter, and B.C. Garrett, Interaction of ClO Radical with Liquid Water, *J. Am. Chem. Soc.*, **131**, 14778-14785 (2009).

405. D.J. Grant, D.A. Dixon, and J.S. Francisco, Heats of Formation of the HX_mY_nH (X=O;Y=S; m,n=0-3) Systems from Electronic Structure Calculations, *J. Phys. Chem. A.*,**113**, 11343-11353 (2009).

404. S. Du and J.S. Francisco, OH-N_2 and SH-N_2 Radical-Molecule Van der Waals Complex, *J. Chem. Phys.*, **131**, 064307 (2009).

403. P.P. Bera, J.S. Francisco, and T.J. Lee, Identifying the Molecular Origin of Global Warming, *J. Phys. Chem. A.*, **113**, 12694-12699 (2009).

402. J.S. Francisco and W. Eisfeld, Atmospheric Oxidation Mechanism of Hydromethyl Hydroperoxide, *J. Phys. Chem. A.,* **113**, 7593 - 7600 (2009).

401. C.J. Christiansen and J.S. Francisco, Atmospheric Oxidation Mechanism of 1,2-Dibromoethane, *J. Phys. Chem. A.*, **113**, 7189 - 7204 (2009).

400. M. Lissmann, B. Hansmann, B. Abel, P. Blachly, and J.S. Francisco, Primary Steps in the Reaction of OH Radicals with Biomolecules at Low Temperatures in Laval Nozzle Expansion Perspectives from Experimental and Theory, *J. Phys. Chem. A.*, **113**, 7570 - 7575 (2009).

399. S. Du, J.S. Francisco, and S. Kais, Study of the Electronic Structure and Dynamics of Interacting Free Radicals Influenced by Water, *J. Chem. Phys.*, **130**,124312 (2009).

398. H.-G. Yu, J.T. Muckerman, and J.S. Francisco, A Theoretical Study of the Reaction of CH_3 with HOCO Radicals, *J. Phys. Chem. A.*, **113**, 3844-3849 (2009).

397. G. Poggi and J.S. Francisco, An Ab Initio Study of the Reaction of HOCO Radicals with NO_2: Addition/Elimination Mechanism, *J. Chem. Phys.*, **130**,124306 (2009).

396. R.J. Buszek and J.S. Francisco, The Gas Phase Decomposition of CF_3OH with Water: A Radical Catalyzed Mechanism, *J. Phys. Chem. A.*, **113**, 5333-5337 (2009).

395. S. Du and J.S. Francisco, Spectroscopic Properties and Stability of the SH-H_2O Open Shell Complex, *J. Chem. Phys.*, **130**, 124304 (2009).

394. J. Franz, J.S. Francisco, S.D. Peyerimhoff, Production of Singlet Oxygen Atoms by Photodissociation of Oxywater, *J. Chem. Phys.*, **130**, 084304 (2009).

393. B.A. O'Donnell, E.X.J. Li, M.I. Lester, and J.S. Francisco, Spectroscopic Identification and Stability of the Intermediate in the OH + $HONO_2$ Reaction, *Proc. Natl. Acad. Sci. USA*, **105**, 12678-12683 (2008).

392. R.M. Ravelo and J.S. Francisco, Proton Affinity of Methyl Nitrite and Methyl Peroxynitrite: Implications for Measuring Branching Ratios of Alkyl Nitrate and Nitrites, *J. Am. Chem. Soc*, **308**, 11234-11239 (2008).

391. H.G. Yu, J.T. Muckerman, G. Poggi, and J.S. Francisco, Energetics and Molecular Dynamics of the Reaction of HOCO with HO_2 Radicals, *J. Chem. Phys.*, **129**, 214307 (2008).

390. K.A. Peterson, D.A. Dixon, and J.S. Francisco, $ClClO_2$ is the Most Stable Isomer of Cl_2O_2. Accurate Coupled Cluster Energetics and Electronic Spectra of Cl_2O_2 Isomers, *J. Phys. Chem. A.*, **112**, 9623-9627 (2008).

389. H.-G. Yu, J.S. Francisco, and J.T. Muckerman, Ab Initio and Direct Dynamics Study of the Reaction of HOCO with Cl Atoms, *J. Chem. Phys.*, **129**, 064301 (2008).

388. H.-G. Yu, J.T. Muckerman, and J.S. Francisco, Energetics and Kinetics of the Reaction of HOCO with Hydrogen Atoms, *J. Chem. Phys.*, **128**, 244315 (2008).

387. J. Matthews, M. Martinez-Aviles, J.S. Francisco, and A. Sinha, Probing OH Stretching Overtones of CH_3OOH Through Action Spectroscopy: Influence of Transition Dipole Moment Dependence on HOOC Torsion, *J. Chem. Phys.*, **129**, 074316 (2008).

386. M. Martinez-Aviles, C.M. Rosedo-Reyes, and J.S. Francisco, Atmospheric Oxidation Mechanism of Bromopropane, *J. Phys. Chem. A.*, **112**, 7930-7938 (2008)

385. S. Du, K.A. Peterson, and J.S. Francisco, Determination of the Rate Constant for Sulfur Recombination by Quasiclassical Trajectory Calculations, *J. Chem. Phys.*, **128**, 204306 (2008).

384. W. Eisfeld and J.S. Francisco, Excited States of Hydroxymethyl Hydroperoxide, *J. Chem. Phys.*, **128**, 174304 (2008).

383. S. Du and J.S. Francisco, Interaction between OH Radical and the Water Interface, *J. Phys. Chem. A.*, **112**, 4826-4835 (2008).

382. J. Switzer, D.J. Grant, M.H. Matus, D.A. Dixon, and J.S. Francisco, Bond Dissociation Energies in Second Row Compounds, *J. Phys. Chem. A.*, **112**, 3145-3156 (2008).

381. D.J. Grant, D.A. Dixon, A.E. Kemeny and J.S. Francisco, On the Structure and Heat of Formation of the Neutral and Ionic PNO, NOP, and PON Systems from Electronic Structure Calculations, *J. Chem. Phys.*, **128**, 164305 (2008).

380. K.A. Peterson, A. Mitrushchenkos and J.S. Francisco, A Theoretical Study of the Spectroscopic Properties of the Ground and First Excited Lowest Two Electronic States of HS_2, *Chem. Phys*., (Invited) **346**, 34-44 (2008).

379. M. Martinez-Aviles, S. Yang, and J.S. Francisco, Structure and Vibrational Spectra of Bromine Reservoir Species from the Atmospheric Oxidations of Bromoethane and Bromopropane, *Mol*. *Phys*.,(Invited) **106**, **299**-314 (2008).

378. S. Du, J.S. Francisco, G.K. Schenter, and B.C. Garrett, Many-Body Decomposition of the Binding Energies for $OH(H_2O)_2$ and $OH(H_2O)_3$ Complexes, *J. Chem. Phys*., **128**, 084307 (2008).

377. J.A.W. Harkless and J.S. Francisco, Bond Dissociations and Conformational Energetics of Tetrasulfur: a Quantum Monte Carlo Study, *J. Phys. Chem. A,* **112**, 2088-2092 (2008).

376. R.M. Ravelo and J.S. Francisco, Proton Affinity of Methyl Peroxynitrate, *J. Phys. Chem*. A, **112**, 1981-1985 (2008).

375. J. Clark, A. Mower, J. Hansen, and J.S. Francisco, Computational Study on the Existence of Organic Peroxy Radical-Water Complexes (RO_2-H_2O), *J. Phys. Chem. A*, **112**, 1587-1595 (2008).

374. H. Beckers, P. Garcia, H. Willner, G.A. Arguello, C.J. Cobos, and J.S. Francisco, Matrix Isolation and ab initio study of FSO_5. A Molecular Complex that Contains 4 Catenated Oxygen Atoms, *Angew. Chem. Int. Ed.*, **46**, 3754-3757 (2007).

373. E. Vohringer-Martinez, B. Hansmann, H. Hernandez, J.S. Francisco, J. Troe, and B. Abel, Water Catalysis of a Radical-Molecule Gas Phase Reaction, *Science*, **315**, 497-501 (2007).

372. M. Martinez-Aviles, C.M. Rosado-Reyes, and J.S. Francisco, Atmospheric Oxidation Mechanism of Bromoethane, *J. Phys. Chem. A*., **111,** 11652-11660 (2007).

371. H. Hernandez, F. Weinhold and J.S. Francisco, Radical Hydrogen Bonding: Origin of Stability of Radical-Molecule Complexes, *J. Chem. Phys.*, **127**, 164102 (2007).

370. H.-G. Yu, J.T. Muckerman, and J.S. Francisco, Quantum Force Molecular Dynamics Study of the O+HOCO Reaction, *J. Chem. Phys.*, **127**, 094301 (2007).

369. K.K. Irikura and J.S. Francisco, Competition Between Hydrogen Abstraction and Halogen Displacement Reaction of Br Atoms with CH_3X (where X=Cl, Br and I), *J. Phys. Chem. A*., **111**, 6852-6859 (2007).

368. J.S. Francisco, Sulfur Atom Exchange in Reactions of SH Radicals with S Atoms, *J. Chem. Phys*., **126**, 214301 (2007).

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366. M.H. Matus, D.A. Dixon, K.A. Peterson, J.A.W. Harkless, and J.S. Francisco, A Coupled- Cluster Theory Study of the Electronic Structure and Energetics of Tetrasulfur, S_4, *J. Chem. Phys.*, **127**, 174305 (2007).

365. S. Du, J.S. Francisco, G.K. Schenter, and B. Garrett, Ab Initio and analytical intermolecular potential for ClO-H_2O, *J. Chem. Phys.*, **126**, 114304 (2007).

364. C.M. Rosado-Reyes and J.S. Francisco, Atmospheric Oxidation Pathways of Propane and its By-Products: Acetone, Acetaldehyde, and Propionaldehyde, *J. Geophys. Res. Atmosphere*, **112**, D14310 (2007).

363. G. Poggi and J.S. Francisco, Hydrogen Atom Abstraction from HOOOCl by Chlorine Atom and OH Radical, *Inorg. Chimi. Acta.* (Invited), **360**, 837-831 (2007).

362. S. Guha and J.S. Francisco, Ab Initio Study of the Structures, Vibrational Spectrum and Energetics of Aluminum Hydrosulfide, *Astrophysical J*., **671**, 2159-2163 (2007).

361. J.D. Watts and J.S. Francisco, Ground and Electronically Excited States of Methyl Hydroperoxide, *J. Chem. Phys*., **125**, 104301 (2006).

360. K.A. Peterson, J.S. Francisco, and J.R. Lyons, Excited States for S_3, *J. Chem. Phys*., **125**, 084314 (2006).

359. J.R. Greene, J.S. Francisco, J. Huang, D. Xu, and W.M. Jackson, Ultraviolet Photodissociation of CBr_4 at 267 nm Using Ion Velocity Imaging, *J. Chem. Phys*., **125**, 133311 (2006).

358. S. Du, J.S. Francisco, G.K. Schenter, T.D. Iordanov, B. Garrett, M. Dupuis, and J. Li, The OH Radical-H_2O Molecular Interaction Potential, *J. Chem. Phys*., **124**, 224317 (2006).

357. C.M. Rosado-Reyes and J.S. Francisco, Atmospheric Oxidation Pathways of Acetic Acid, *J. Phys. Chem. A*, **110**, 4419-4433 (2006).

356. J.S. Francisco and J.N. Crowley, A Theoretical Investigation of Product Channels in the CH_3O_2 + Br Reaction, *J. Phys. Chem A*., **110**, 6948-6959 (2006).

355. J.S. Francisco, Ab Initio Study of the Structure, Vibrational Spectra, and Energetics of XBS^+ (where X=H, F, and Cl), *J. Chem. Phys*., **124**, 114303 (2006).

354. L. Christensen, J.C. Hansen, M. Okumura, S.P. Sander and J.S. Francisco, Experimental and Ab Initio Study of the HO_2-CH_3OH Complex: Thermodynamics and Kinetics of Formation, *J. Phys. Chem. A*., **110**, 3778-3784 (2006).

353. D.A. Dixon, J.S. Francisco, and Y. Alexeev, Thermochemical Properteis of NOH_x Molecules and Ions from Ab Initio Electronic Structure Theory, *J. Phys. Chem. A*., **110**, 185-191 (2006).

352. J.M.C. Plane, D.M. Joseph, B.J. Allan, S.H. Ashworth, and J.S. Francisco, An Experimental and Theoretical Study of the Reactions OIO+NO and OIO+OH, *J. Phys. Chem. A*, **110**, 93-100 (2006).

351. Y. Li and J.S. Francisco, Mechanism for the Hydrolysis of Peroxyacetyl Nitrate (PAN): The Importance of the Second Water Molecule, *J. Am. Chem. Soc*., **127**, 12144-12146 (2005).

350. J. Matthews, A. Sinha, and J.S. Francisco, The Importance of Weak Absorption Features to Contributions in Tropospheric Radical Production, *Proc. Natl. Acad. Sci. USA*., **102**, 7449-7452 (2005).

349 B. Suitte, S.D. Belair, and J.S. Francisco, Spectroscopic Characterization of the Five Possible Orientations of a Hydrogen Bonded Pair of Water Molecules within Cubic Water Octamer Framework, *Phys. Rev. A*., **71**, 043204 (2005).

348. J.S. Francisco, J.R. Lyons, and I.H. Williams, High Level ab Initio Studies of the Structure, Vibrational Spectra and Energetics of S_3, *J. Chem. Phys*., **123**, 054302 (2005).

347. H.-G. Yu, J.T. Muckerman, and J.S. Francisco, Direct ab Initio Dynamics Study of the OH+HOCO Reaction, *J. Phys. Chem. A.*, **109**, 5230-5236 (2005).

346. Q. Shi, S. Kais and J.S. Francisco, Graph Theory for Fused Cubic Clusters of Water Dodecamer, *J. Phys. Chem. A*, **109**, 12036-12045 (2005).

345. D.J. Goebbert, H. Hernandez, J.S. Francisco, and P.G. Wenthold, The Binding Energy and Bonding in Dialane, *J. Am. Chem.. Soc*., **127**, 11684-11689 (2005).

344. C.M. Rosado-Reyes, J.S. Francisco, J.J. Szente, M.M. Maricq, and L.F. Oestergaard, Dimethyl Ether Oxidation at Elevated Temperatures, *J. Phys. Chem. A*, **109**, 10940-10953 (2005).

343. J. Matthews, A. Sinha, and J. S. Francisco, Unimolecular Dissociation of CH_3OOH, *J. Chem. Phys*., **122**, 221101 (2005).

342. S. von Ahsen and J.S. Francisco, Spectroscopic Evidence for the Existence of the CF_3OSO_3 Radical, *J. Phys. Chem. A*., **109**, 9193-9195 (2005).

341. M. Schnell, J.S. Francisco, and S. Peyerimhoff, Electronic Excited State Potential Energy Surfaces for HOOOCl, *Phys. Chem. Chem. Phys*., **7**, 1912-1917 (2005).

340. A.B. McCoy, J.L. Fry, J.S. Francisco, S.P. Sander, A.K. Mollner, and M.Okamura, Theoretical and Experimental Investigation of the First Overtone Spectrum of cis-cis HOONO: The Role of OH-Stretch/Torsion Coupling and Quantum Yield Effects, *J. Chem. Phys*., **122**, 104311 (2005).

339. E.S. Whitney, A.M. Zolot, A.B. McCoy, J.S. Francisco, and D.J. Nesbitt, Simple Impulsive Model Reactive Scattering Dynamics in Atom + Polyatomic Systems: $F+C_2H_6 \rightarrow HF(v,J)+C_2H_5$, *J. Chem. Phys.*, **122**, 124310 (2005).

338. S.D. Belair, J.S. Francisco, and S.J. Singer, Hydrogen Bonding in Cubic $(H_2O)_8$ and $OH\bullet(H_2O)_7$ Clusters, *Phys. Rev. A*., **71**, 013204 (2005).

337. M. Kronberg, S. von Ahsen, H. Willner and J.S. Francisco, Spectroscopic Characteristic of SF_5O_x Radicals (x=0-3), *Angew. Chem. Int. Ed*., **44**, 253-257 (2005).

D. Published Reports and Book Reviews:

15. J.S. Francisco, Chair; et al. *Challenges in Chemistry Graduate Education: A Workshop Summary*, Committee on Challenges in Chemistry Graduate Education, Board of Chemical Sciences and Technology, National Research Council, Washington, National Academy Press, pp 1-86 (2012).
14. J.S. Francisco, "Challenging Times Require Fresh Approaches to Job Creation", *C&EN News*, **89,** no. 23, 44 (2011).
13. J.S. Francisco and J.L. Benham, "Globalization, Opportunities, Readiness, and ACS – ACS International Center", *C&EN News*, **89,** no. 20, 38 (2011).
12. J.S. Francisco, "A New Frontier in Atmospheric Chemistry: Computational Atmospheric Chemistry", *Computational and Theoretical Chemistry*, **965**, 248 (2011).
11. J. S. Francisco and B.A. Charpentier, "A Fresh Look at ACS Dues and Member Benefits", *C&EN News*, **89**, no. 7, 40 (2011).
10. J.S. Francisco and J.I. Steinfeld, "Educating for Sustainability*", C&EN News*, **88**, no. 38, 32 (2010).
9. T.H. Lane and J.S. Francisco, "Building A Diverse Profession and Inclusive Community", *C&EN News*, **88,** no. 25, 35 (2010).
8. J.S. Francisco and T.A. Ring, "Who Is Missing From the Table?", *C&EN News*, **88,** no. 17, 48 (2010).
7. J.S. Francisco, To Be Competitive, You Need a Global Education, *In Chemistry*, **19**, 2 (2010).
6. J.S. Francisco, Chemistry in a Global Economy – An Education Agenda, *J. Chem. Educ*., **85**, 1338 (2008).
5. C.P. Casey, J.S. Francisco, and T. Masciangioli, National Research Council Report, "The Future of U.S. Chemistry Research: Benchmarks and Challenges", *J. Chem. Educ*., **84**, 1089 (2007).
4. J.S. Francisco, Looking at History for Inspiration: The Achievements of Percy L. Julian, *In Chemistry*, 16, 11-13 (2007).

3. J.S. Francisco, review of "Unimolecular Reactions", W. Frost, *Chem. Phys. Chem.*, 5, 1251 (2004).
2. J.S. Francisco, review of "Reviews on Computational Chemistry, Volume 19", *J. Am. Chem. Soc.*, 126, 3003 (2004).
1. J.S. Francisco and I.M. Warner, "Minorities in the Chemical Workforce: Diversity Models that Work", National Academy Press (2003), pp. 1-174.

PAPERS PRESENTED

A. Invited and/or refereed internationally or nationally (Total 106, those since 2005 listed below):

106. Plenary and Keynote Speaker, North Carolina A&T University, Biennial Chemical Sciences Symposium, Greensboro, NC, October 31, 2014
105. Invited Speaker, American Conference of Theoretical Chemistry (ACTC), Telluride, CO, July 21-24, 2014.
104. Invited Speaker, Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride, CO, July 7-13, 2014.
103. Plenary Speaker, 25th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX, March 1-4, 2014.
102. Invited Speaker, Symposium on "New Chemical Frontiers in Solar System Exploration", American Chemical Society, Indianapolis, IN, September 8-12, 2013.
101. Keynote Speaker, 20th Anniversary of the Committee of Minority Affairs, American Chemical Society, Indianapolis, IN, September 9, 2013.
100. Invited Speaker, Symposium on "Morrill Act Symposium", American Chemical Society, Philadelphia, PA, August 19, 2012.
99. Plenary Speaker, Biannual Conference on Chemical Education, Pennsylvania State University, University Park, PA , July 30, 2012.
98. Invited Speaker, Spectroscopy and Dynamics on Multiple Potential Energy Surfaces, Telluride, CO, July 9-13, 2012.
97. Plenary Speaker, Peter Anthony Leermakers Symposium, Wesleyan University, Middletown, CT, May 12, 2012.
96. Plenary Speaker, CFCAM Workshop on Anharmonicity in Medium-Sized Molecules on Clusters, Paris, France, April 18-21, 2012.
95. Invited Speaker, NASA Astrobiology Science Conference 2012, "The Role of Quantum Chemistry in Astronomical and Astrobiological Context", Atlanta, GA, April 16-20, 2012.
94. Invited Speaker, Symposium on "Inspiring Science Education: Readiness for the Global Enterprise", American Chemical Society, San Diego, CA, March 26, 2012.
93. Plenary Speaker, Dallas Symposium on Molecular Structure and Dynamics, Dallas, TX, March 3-6, 2012.
92. Invited Speaker, Humboldt Kolleg: Collaborations and Networks in the 21st Century, Arlington, VI, February 24-25, 2012.
91. Keynote Speaker, Second International Workshop on Spectroscopic Signatures of Molecular Complexes/Ions in Our Atmosphere and Beyond, Varanasi, India, February 7-10, 2012.
90. Invited Speaker, Gordon Conference on Molecular Ionic Clusters, Ventura, CA, January 29 – February 2, 2012.
89. Keynote Speaker, Midwest Astrochemistry Meeting, Urbana-Champaign, IL October 21-22, 2011
88. Plenary Speaker, 20th Anniversary of the Centre De Supercomputacio De Catalunya, "Chemistry Computation and Society", Barcelona, Spain, October 15-19, 2011.
87. Plenary Speaker, 46th Meeting of the Mexican Chemical Society (Sociedad Quimica de Mexico, SQM), Queretaro, Mexico, September 10-14, 2011.

86. Invited Speaker, GDCh-Wissenschaftsforum Chemie, Bremen, Germany, September 4-7, 2011.
85. Invited Speaker, Symposium on "ACS Past Presidents", American Chemical Society, Denver, CO, August 28- September 1, 2011.
84. Invited Speaker, Symposium on "Air-Surface Interactions: Chemistry from Molecular to Global Climate Scales", American Chemical Society, Denver, CO, August 28-September 1, 2011.
83. Invited Speaker, Ninth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC), Santiago de Compostela, Spain, July 17-22, 2011.
82. Plenary Speaker, LaTroisieme Journee Interntionale de Modelisation Quantique et de Nanomateriaux, Tunis, Tunisia, July 12-15,2011.
81. MPS Distinguished Lecture, Mathematical and Physical Science Division, National Science Foundation, Washington, D.C. May 16, 2011.
80. Invited Speaker, Symposium on "International Collaboration in the Chemical Sciences: Best Practices", American Chemical Society, Anaheim, CA, March 28, 2011.
79. Invited Speaker, Symposium on "75 Years of CPT: It's Not Just About Approval", American Chemical Society, Anaheim, CA, March 27, 2011.
78. Invited Speaker, 2011 Southeast Chemistry Department Chairs Meeting, Mississippi State University, Starksville, MS, March 18-19, 2011.
77. Invited Speaker, 7th AirUCI Annual Workshop Program, Laguna Beach, CA, January 25, 2011.
76. Invited Speaker, Pacifichem 2010, Symposium on Free Radical Chemistry in the Environment, Honolulu, HI, December 15-20, 2010.
75. Distinguished Lise Meitner-Fellow Lecturer, Lise-Meitner Symposium, Jerusalem, Israel, November 21, 2010.
74. Keynote Speaker, 34th ACS Senior Technical Meeting, Puerto Rico Local Section, Mayaquez, Puerto Rico, November 5, 2010.
73. Keynote Speaker, 8th International Conference and Exhibition on Chemistry in Industry, Manama, Kingdom of Bahrain, October 18-20, 2010.
72. Invited Speaker, Symposium on "Physical Chemistry of Hydrates, Interfaces and Aerosols and Their Relationship to the Climate System", American Chemical Society, Boston, MA, August 22-26, 2010.
71. Invited Speaker, 21st International Conference on Chemical Education (21st ICCE), Taipei, Taiwan, August 8-13, 2010.
70. Plenary Speaker, 2010 Tri-State Chinese American Chemical Society Annual Symposium on "Opportunity for Chemistry in a New Decade – Its Impact On and Around Us", Rutgers University, Piscataway, NJ, June 26, 2010
69. Invited Speaker, 93rd Canadian Chemistry Conference and Exhibition, Toronto, Canada, May 29-June 3, 2010.
68. Invited Speaker, Centennial Celebration of Chemical Research and Education, Peking University, Bejing, China, May 3, 2010.
67. Plenary Lecture, Korean Chemical Society 105th National Meeting, Inchon, Korea, April 29-30, 2010.
66. Invited Speaker, Solvay Workshop on "Molecular Complexes in Our Atmosphere and Beyond", Solvay Institute, Universite Libre de Bruxelles, Belgium, April 20-23, 2010.
65. Plenary Speaker, 6th Annual Poe Symposium on "Climate Change in the 21th Century", California State University Channel Islands, Camarillo, CA, April 16, 2010.
64. Invited Speaker, Nanomaterials and Nanocatalysis for Energy, Petrochemicals and Environmental Applications, Cairo, Egypt, March 27-April 7, 2010.
63. Invited Speaker, Symposium on "Dynamics in Clusters and Floppy Systems: Theory and Experiment", American Chemical Society, San Francisco, March 21-25, 2010.
62. Invited Speaker, Symposium on "Chemical Education at a Crossroads", American Chemical Society, Washington, DC, August 16-20, 2009.

61. Keynote Speaker, Symposium on "Enhancing Diversity at the Graduate and Postdoctoral Levels",American Chemical Society, Washington, DC, August 16-20, 2009.
60. Plenary Speaker, SACNAS Leadership Program, Washington, DC, July 27-29, 2009.
59. Plenary Speaker, Theoretical Chemistry: Modeling Reactivity from Gas Phase to Biomolecules and Solids, Celebrating 25 years of Theoretical Chemistry in Catalonia, Spain," Barcelona, Spain, June 29-July 3, 2009.
58. Invited Speaker, Symposium on "Current Practices in Understanding Atmospheric Chemistry", American Chemical Society, Salt Lake City, Utah, March 23-25, 2009.
57. Keynote Speaker, Workshop on Excellence Empowered by a Diverse Academic Workforce: Chemists, Chemical Engineers and Material Scientists with Disabilities, Arlington, Virginia, February 8-10, 2009.
56. Invited Keynote Speaker, IGAC-SPARC Workshop on Atmospheric Chemical Kinetics, Cambridge England, June 19-20, 2008.
55. Plenary Speaker, Ninth Informal Conference on Atmospheric and Molecular Science, Helsingor, Denmark, June 6-8, 2008.
54. Invited Speaker, Symposium on "Electronic Structure and Reaction Dynamics of Open-Shell Species", American Chemical Society 235th National Meeting, New Orleans, LA, April 6-10, 2008.
53. Plenary Speaker, Tuskegee University Mentoring Workshop, Tuskegee University, Tuskegee, Alabama, March 15, 2008.
52. Invited Speaker, Singapore International Chemistry Conference 5, Singapore City, Singapore, December 16-19, 2007.
51. Invited Speaker, 29th International Symposium on Free Radicals, Big Sky Montana, August 12-17, 2007.
50. Keynote Speaker, 6th Annual Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY), Hamilton College, Clinton, NY, July 29-31, 2007.
49. Invited Speaker, Joint Assembly of the American Geophysical Union, Symposium on Atmospheric Aerosol Processes, Acapulco, Mexico, May 22-25, 2007.
48. Plenary Speaker, Tampa Bay ACS Local Section Annual Meeting-in-Miniature, St. Petersburg, FL, March 9, 2007.
47. Keynote Speaker, Presidential Symposium Honoring Percy Julian, American Chemical Society 232nd National Meeting, San Francisco, September 12, 2006.
46. Invited Speaker, Symposium on "Cyber-Enabled Chemistry", American Chemical Society 232nd National Meeting, San Francisco, September 10-14, 2006.
45. Invited Speaker, Telluride Workshop on Molecular Aspects of Solvation in Hydrogen Bonded Systems", Telluride, CO, August 7-11, 2006.
44. Keynote Speaker, Pinhead Town Talk, Pinhead Institute, Telluride, CO, August 8, 2006.
43. Invited Speaker, Symposium on "Emerging Issues in Atmospheric Science", American Chemical Society 231st National Meeting, Atlanta, GA, March 26-30, 2006.
42. Invited Speaker, Gordon Conference on Molecular Ionic Clusters, Ventura, CA, February 19-24, 2006.
41. Keynote Speaker, Alliance for Graduate Education in Mississippi Winter Symposium, Hattiesburg, MS, January 19-21, 2006.
40. Invited Speaker, Pacifichem 2005, Symposium on Free Radical Chemistry in the Environment, Honolulu, HI, December 15-20, 2005.
39. Invited Speaker, Symposium on "Theoretical Determination of Energy Landscapes: Methodology and Application", American Chemical Society 230th National Meeting, Washington, D.C., August 28-Sept. 1, 2005.
38. Invited Speaker, Asian-Pacific Combustion Conference, Adelaide, Australia, July 17-20, 2005.

37. Keynote Speaker, F.E. Mapp Symposium, Morehouse College, Atlanta, Georgia, April 12, 2005.
36. Invited Speaker, Session on "Atmospheric and Planetary Sciences", National Organization of Black Chemists and Chemical Engineers, Orlando, FL, March 20-26, 2005.
35. Invited Speaker, Symposium on "The Rise and Fall of Chlorofluorocarbons", American Chemical Society, 229th National Meeting, San Diego, CA, March 13-17, 2005.

B. Invited Seminars or Invited Lectures (Total 328, those since 2005 presented below):

328. Grinnell College, Department of Chemistry (Danforth Lecture), Grinnell, IA, April 2014
327. Argonne National Laboratory, Chemical Sciences and Engineering Division Colloquium, April 15, 2014.
326. Indiana University, Department of Chemistry, Bloomington, IN, October 31, 2013.
325. University of North Texas, Department of Chemistry, Denton, TX, October 11, 2013.
324. University of Nebraska-Lincoln, Department of Chemistry (Chair Lecture), Lincoln, NE, October 5, 2013.
323. Qatar Environment and Energy Research Institute, Doha, Qatar, May 27, 2013.
322. Western Washington University, Department of Chemistry (Scholars Day Distinguished Keynote Speaker), Bellingham, WA, May 15-17, 2013.
321. University of Northern Colorado, Department of Chemistry and Biochemistry, Greely, CO, April 19, 2013.
320. Brown University, Department of Chemistry, Providence, RI, March 8, 2013.
319. University of Connecticut, Department of Chemistry and Physics, Storrs, CT, March 7, 2013.
318. University of Texas at San Antonio, Department of Chemistry, San Antonio, TX, March 1, 2013.
317. Dominican University of California, Department of Chemistry, San Rafael, CA, February 7, 2013.
316. University of Georgia, Department of Chemistry (Charles A. Coulson Lecture), Athens, GA, November 27, 2012.
315. Forschungszentrum Juelich, Institute of Energy and Climate Research, Juelich, Germany, October 25, 2012.
314. University of Wuppertal, Institute of Physical Chemistry, Wuppertal, Germany, June 29, 2012.
313. Uppsala University, Department of Chemistry, Uppsala, Sweden, June 20, 2012.
312. University of Colorado, Department of Chemistry and Biochemistry (Physical Chemistry/Chemical Physics Colloquium), Boulder, CO, May 4, 2012.
311. University of Pennsylvania, Department of Chemistry (Inaugural NOBCChE Lecture), Philadelphia, PA, April 26, 2012.
310. Wabash Valley ACS Local Section, Rose-Hulman Institute of Technology, Terra Haute, IN April 10, 2012.
309. Mississippi State University, Department of Chemistry, Starksville, MS, March 23, 2012
308. Proctor and Gamble, Innovation Lecture Series, Cincinnati, OH, March 9, 2012
307. Louisiana State University, Department of Chemistry (Colloquium), Baton Rouge, LA, March 2, 2012
306. BASF – The Chemical Company, Innovation Lecture Series, Newark, NJ, February 27, 2012
305. NOAA, Earth Systems Research Laboratory, Chemical Science Division, Boulder, CO, December 14, 2011.

304. Laboratory for Atmospheric and Climate Science, National Scientific Research Council (CSIC) Toledo, Spain, October 29, 2011.
303. Georgia Southwestern State University, Department of Chemistry, Americus, GA, October 5, 2011.
302. University of South Florida, Department of Chemistry (Martin Lecture), St. Petersburg, FL, September 22, 2011.
301. Universite Henri Poincare, Equipe de Chimie et Biochimie Theoriques, Vandoeuvre-les-Nancy, France, July 8, 2011.
300. Ecole Normale Superleure, Departement de Chimie, Paris, France, July 4, 2011.
299. Universite Lyon, Institut de Recherches sur la Catalyse et l'Environnement , Lyon, France, June 15, 2011.
298 Universite Paris-Est, Laboratoire de Modelisation et Simulation Multi Eschelle, Marne la Vallee, France, June 24, 2011.
297. Central Region ACS (CERM) Meeting (Keynote Speaker), Indianapolis, IN, June 8, 2011.
296. Case Western Reserve University, Department of Chemistry, Cleveland, Ohio, June 2, 2011.
295. Joint Cleveland Section ACS/Society for Applied Spectroscopy Meeting (Keynote Speaker), Cleveland, Ohio, June 1, 2011.
294. University of Arkansas, Department of Chemistry, Little Rock, AR, May 20, 2011.
293. BASF – The Chemical Company, Innovation Lecture Series, Research Triangle Park, NC, April 29, 2011.
292. Lehigh Valley ACS Local Section, Bethlehem, PA, April 26, 2011.
291. Illinois Institute of Technology, Department of Chemistry, Chicago, Il, April 14, 2011.
290. Yeshiva University, Department of Chemistry, New York, NY, April 10, 2011.
289. Edinboro University of Pennsylvania, Department of Chemistry, Edinboro, PA, April 8, 2011.
288. Pennsylvania State University, Department of Chemistry (Colloquium), University Park, PA, April 7, 2011.
287. Nashville Local Section ACS (Plenary Speaker), Nashville, TN, March 22, 2011.
286. BASF – The Chemical Company, Innovation Lecture Series, Wyandotte, MI, March 15, 2011.
285. University of Alabama at Birmingham, Department of Chemistry, Birmingham, AL, March 10, 2011.
284. Virginia Tech, Department of Chemistry, Blacksburg, VI, March 4, 2011.
283. Purdue University, Department of Chemical Engineering, January 18, 2011.
282. Technion Institute of Technology, Department of Chemistry, Haifa, Israel, November 24, 2010.
281. Hebrew University (Distinguished Lise Meitner-Fellow Lectureship), Department of Chemistry, Jerusalem, Israel, November 21, 2010.
280. Tuskegee University, Department of Chemistry, Tuskegee, AL, September 13, 2010.
279. University of Oslo, Center for Theoretical and Computational Chemistry, Oslo, Norway, September 4, 2010.
278. National Taiwan University, Department of Chemistry, Taipei, Taiwan, August 12, 2010.

277. Imperial College (University of London), Department of Chemistry, London, England, July 6, 2010.
276. University of Texas at Austin, Department of Chemistry, Austin, TX, May 20, 2010.
275. NASA-Ames Research Center (Director's Colloquium), Moffett Field, CA, May 11, 2010.
274. Pohang University of Science and Technology, School of Environmental Science and Engineering, Pohang, Korea, April 28, 2010.
273. Seoul National University, Department of Chemistry, Seoul, Korea, April 27, 2010.
272. National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (Henry A. Hill Lecture), Atlanta, GA; March 30, 2010
271. St. Johns University, Department of Chemistry, Queens, New York, March 4, 2010.
270. Johns Hopkins University, Applied Physics Laboratory Colloquium, Baltimore, MD, February 25, 2010.
269. Chemical Society of Washington, Washington, DC, January 14, 2010.
268. Cornell University, Department of Chemistry and Chemical Biology, Ithaca, NY, January 12, 2010
267. Purdue University, Department of Computer Science, West Lafayette, IN, December 10, 2009.
266. Brigham Young University, Department of Chemistry (Visiting Distinguished Lecture), Provo, UT, December 7-8, 2009.
265. Northwestern University, Department of Chemistry (L. Carroll King Memorial Lecture), Evanston, Il, November 23 -24, 2009.
264. University of Copenhagen, Department of Chemistry, Copenhagen, Denmark, November 20, 2009.
263 Universite Paris-Est, Laboratoire de Modelisation et Simulation Multi Eschelle, Marne la Vallee, France, November 18, 2009.
262. Universite Henri Poincare, Equipe de Chimie et Biochimie Theoriques, Vandoeuvre-les-Nancy, France, November, 17, 2009.
261. University of Leipzig, Institute of Physical Chemistry, Leipzig, Germany, November 12, 2009.
260. Southwest Regional ACS Meeting (Plenary Lecture), El Paso, TX, November 8, 2009.
259. Midwest Regional ACS Meeting (Presidential Plenary Lecture), Iowa City, Iowa, October 21-24 2009.
258. Columbus Local ACS Meeting (Keynote Speaker), Columbus, Ohio, October 20, 2009.
257. Northeast Regional ACS Meeting (NERM 2009), Hartford, Conn, October 7-10, 2009.
256. University of North Carolina-Asheville, Department of Chemistry (S. Dexter Squibb, Distinguished Lecture), Asheville, NC, October 1-2, 2009.
255. M.I.T, Department of Chemistry, Cambridge, MA, September 28, 2009.
254. Xavier University, Department of Chemistry, New Orleans, LA, September 17, 2009.
253. Universitat de Barcelona, Facultat de Quimica, Barcelona, Spain, July 6, 2009.
252. South Florida Section ACS (Plenary Speaker), Miami, FL, April 18, 2009.

251. Florida International University, Department of Chemistry, Miami, FL, April 17, 2009.
250. Cincinnati Section ACS (Plenary Speaker), Cincinnati, OH, December 4, 2008.
249. Virginia Commonwealth University, Department of Chemistry, Richmond, VA, November 6, 2008.
248. University of Wisconsin, Department of Chemistry, Madison, WI, October 28, 2008.
247. University of California at Riverside, Department of Chemistry, Riverside, October 8, 2008.
246. University of California at Irvine, Department of Chemistry, Irvine, CA, October 7, 2008.
245. Auburn University, Department of Chemistry, Auburn, AL, September 18, 2008.
244. University of Lund, Department of Chemistry, Lund, Sweden, June 5. 2008.
243. University of Gottingen, Institute of Physical Chemistry, Gottingen, Germany, June 2, 2008.
242. Radboud University of Nijmegen, Theoretical Chemistry Institute for Molecules and Materials, Nijmegen, Netherlands, May 30, 2008.
241. Scripps Institute of Oceanography, Center for Atmospheric Science, LaJolla, CA, May 13, 2008.
240. University of California at San Diego, Department of Chemistry, LaJolla, CA, May 12, 2008.
239. Telluride Pinhead Institute Scholar Lectureship, Telluride, CO, May 5-7, 2008
238. Texas Southern University, Department of Chemistry, March 12, 2008.
237. Wilkes University, Distinguished Speaker, Wilkes-Barre, PA, January 18, 2008.
236. National University of Singapore, Department of Chemical and Biochemical Engineering, Singapore City, Singapore, December 17, 2007.
235. University of the Pacific, Department of Chemistry, Stockton, CA, December 11, 2007.
234. University of Texas at Austin, College of Natural Science, (Distinguished Speaker Series), Austin, TX, November 9, 2007.
233. University of Texas at Austin, Department of Chemistry (Analytical and Physical), Austin, TX, November 8, 2007.
232. University of Freiburg, Department of Geoscience, Freiburg, Germany, October 22, 2007.
231. University of Bielefeld, Department of Theoretical Chemistry, Bielefeld, Germany, October 18, 2007.
230. Purdue University, McCoy Distinguished Lecture, West Lafayette, IN, October 10, 2007.
229. Emory University, Department of Chemistry, Atlanta, GA, May 16, 2007.
228. University of Oregon, Department of Chemistry, Eugene, OR, May 7, 2007.
227. University of Maryland, Department of Chemistry, College Park, MD, April 26, 2007.
226. Clark Atlanta University, Department of Chemistry, Atlanta, GA, April 17, 2007.
225. University of California at Berkeley, Symposium in Honor of William A. Lester 70th Birthday, Department of Chemistry, Berkeley, CA, March 28, 2007.
224. Clemson University, Department of Chemistry, Clemson, SC, March 15, 2007.

223. Andrews University, Department of Chemistry & Biochemistry, Berrien Springs, MI, January 18, 2007.
222. University of Illinois, Department of Chemistry, Urbana-Champaign, IL, December 6, 2006.
221. Loyola University, Department of Chemistry, Chicago, IL, November, 16, 2006.
220. Louisiana State University, Department of Chemical Engineering, Baton Rouge, LA, November 10, 2006.
219. Corning Corporation, Science and Technology Division, Corning, NY, June 14, 2006.
218. Spelman College, Department of Chemistry, Atlanta, GA, April 20, 2006.
217. National Institute of Standards and Technology, Physical and Chemical Properties Division, Gaithersburg, MD, December 8, 2005.
216. McGill University, Department of Chemistry, (McGill Chemical Society Lecture), Montreal, Canada, November 15, 2005.
215. University of California at Los Angeles, Department of Atmospheric and Oceanic Sciences (Atmos. Chemistry Division), November 11, 2005.
214. University of Sydney, Department of Chemistry, Sydney, Australia, July 25, 2005.
213. Universidad Autonoma de Madrid, Departimento de Quimica, Madrid, Spain, May 12, 2005.
212. Universite Bordeaux, CNRS, Laboratoire de Physico-Chimie Moleculaire, Bordeaux, France, May 10, 2005.
211. University of Bremen, Department of Chemistry, Bremen, Germany, May 6, 2005.
210. University of Leipzig, Leibniz-Institut fur Troposphoren Forschung, Leipzig, Germany, May 3, 2005.
209. University of Alabama, Department of Chemistry, Tuscaloosa, AL, April 15, 2005.
208. Washington University, Department of Chemistry, St.Louis, MO, March 3, 2005.
207. Amherst College, Department of Chemistry, Amherst, MA, February 25, 2005.
206. University of Kansas, Department of Chemistry (Departmental Series), Lawrence, KS, February 4, 2005.
205. University of Utah, Department of Chemistry, Salt Lake City, Utah, January 24, 2005.

PROFESSIONAL SERVICE

National Research Council

Elected, Chair, U.S. National Committee for the International Union of Pure and Applied Chemistry, National Research Council, January 1, 2012 – present.

Chair, Organizing Committee for the Workshop on Challenges in Graduate Education, January 23-24, 2012.

Member, National Research Council Board on Science Education, May 21, 2010 – present

Member, National Academies Laboratory Assessments Board, September 28, 2009 – present

Member, Committee on Advancing Institutional Transformation for Minority Women in Academia, June 1, 2011-November 31, 2012.

Elected, Vice Chair, U.S. National Committee for the International Union of Pure and Applied Chemistry, National Research Council, September 14, 2007 – December 31, 2011.

Member, National Academies Panel for Chemical Science and Technology, December 16, 2008 – September 30, 2009.

Member, National Academies Panel for Chemical Science and Technology, March 5, 2007-July 31, 2007.

Appointed, National Research Council Board on Chemical Sciences and Technology, Committee on Benchmarking the Research Competitiveness of US Chemistry, 1 February 2006-31 June, 2006.

Appointed, U.S. National Committee for the International Union of Pure and Applied Chemistry, National Research Council, July 1, 2004-June 30, 2007.

Member, Chemical Sciences Roundtable, National Research Council, January 1, 2001-December 31, 2003.

National Science Foundation

Chair, Committee of Visitors for Chemistry Division National Science Foundation, February 19-21, 2013.

Member, Geosciences Advisory Committee, National Science Foundation, October 14, 2007-present.

Member, Committee of Visitors for Chemistry Division National Science Foundation, February 7-9, 2007.

Member, Committee on Equal Opportunities in Science and Engineering, NSF-Congressionally Mandated Committee, National Science Foundation, 2006-2009, 2009-2012.

Department of Energy

Member, Combustion Site Review Committee, Argonne National Laboratory, Office of Basic Energy Sciences, November 6-8, 2013.

Member, Committee of Visitors for Chemical Sciences, Geosciences, and Biosciences for Department of Energy, Office of Basic Energy Sciences, December 1, 2004 – November 30, 2005.

Department of Defense

Member, Defense Science Study Group, Institute for Defense Analyses, Alexandria, VA, July, 1988 - November, 1991

Member, Senior Science Advisory Committee for the Secretary of the Navy (NRAC), March 31, 1994 - September 1, 1996

Member, Army Research Science Board, Department of Army,
March , 1997 - April, 1999

American Chemical Society

President, American Chemical Society, January 1, 2010 – December 31, 2010.

President-Elect, American Chemical Society, January 1, 2009 – December 31, 2009.

Member, Board of Directors, American Chemical Society, January 1, 2009 – December 31, 2011.

Appointed, Graduate Education Advisory Board of the American Chemical Society, March 1, 2008- December 31, 2008.

Appointed, Committee on Professional Training, American Chemical Society, January 1, 2003 – December 30, 2009.

Consultant, Committee on National Historic Chemical Landmarks, January 18, 2008 – present.

Appointed, ACS Presidential Task Force on Enhancing Innovation and Competitiveness, June 25, 2007.

Appointed, Special Board Task Force on the Review of the ACS National Awards Program, October 23, 2006.

Appointed, ACS Board Oversight Group on Leadership Development, November 8, 2004 – September 30, 2008.

Vice-Chair, American Chemical Society Task Force on Minority Faculty in the Chemical Academic Community, December 1, 2001-December 6, 2002.

Council for Chemical Research

Elected, Board of Directors, Council for Chemical Research, January 1, 2009-December 31, 2010.

Member, Organizing Committee, Council for Chemical Research, July 16, 2007-April 29, 2008.

Council for Scientific Society Presidents

Elected Executive Board, Council for Scientific Society Presidents, December 6, 2009 – December 31, 2010.

Alexander von Humboldt Foundation

Appointed Member, International Advisory Board, November 8, 2013 – present.

Gordon Research Conferences

Elected Member, Board of Trustees, November 1, 2014 – November 1, 2019

National Organization for the Professional Advancement of Black Chemist and Chemical Engineers

Elected President, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, July 1, 2005-June 30, 2007.

Member, Board of Directors, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers, January 1, 2003 – December 31, 2007.

Faculty Advisor for Student Chapter of NOBCChE at Purdue University, September 1995-present.

Organized the First Student Chapter of NOBCChE at Purdue University, September 1995.
Organized the First Student Chapter of NOBCChE at Wayne State University, September 1987.

Faculty Advisor for Student Chapter of the NOBCChE at Wayne State University, September, 1987 - December 1994.

University Visiting Committees

Member, External Review Committee for the Department of University of Utah; November 19, 2013

Member, External Review Committee for the Chemistry Department of Case Western Reserve University; March 19, 2013

Member, University of Texas at Austin, College of Natural Science Foundation Advisory Council, October, 2009 – June, 2011

Member, M. I. T. Corporation Visiting Committee for the Chemistry Department October, 2009 – June 30, 2012

Member, External Review Committee for Chemistry, National Commission for Academic Accreditation and Assessment, King Faisal University, Riyadh, Saudi Arabia, November 14-18, 2008.

Member, External Review Committee for the Chemistry Department of Morehouse College, April 15, 2007-June 1, 2007.

Member, Advisory Board for the MIE Center, Spelman College, January 1, 2003-present.

Member, Advisory Committee for the Center for the Study of Terrestrial and Extraterrestrial Atmospheres at Howard University:
May 17, 1993
October 2, 1993
October 4, 1994
October 6, 1995
September 24, 1997

Chairman, Advisory Board for the Environmental Sciences Institute at Florida A&M University, August 1, 2000-present.

Member, Advisory Committee for the Computational Center for Molecular Structure and Interactions at Jackson State University, March 9, 1999-present.

Member, Senior Advisory Committee for the Material Science Center Subcommittee of the National Advisory Council for Research at Howard University, June 16, 1990 - December 31, 1997.

Member, External Review Committee for the Chemistry Department of Louisiana State University; April 6-8, 1997

Member, M. I. T. Corporation Visiting Committee for the Chemistry Department for the period:
October, 1987 - June 30, 1990
October, 1990 - June 30, 1992
October, 1992 - June 30, 1994
October, 1994 - June 30, 1996

Organization of Scientific Conferences

8. Chair and Co-organizer, Workshop on "Challenges in Graduate Education" for the Board on Chemical Sciences and Technology, National Research Council, January 23-24, 2012

7. Co-organizer, Symposium on “Free Radicals in the Environment”, Pacifichem 2005, Honolulu, HI, December 15-20, 2005.

6. Co-organizer, Presidential Symposium on “Global Climate Change”, American Chemical Society 227th National Meeting, New York, NY, September 7, 2003.

5. Co-organizer, Symposium on “Theoretical Chemistry Applied to the Environment”, the 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry, Ottawa, Canada, August 10-15, 2003.

4. Co-organizer, Workshop on "Minorities in the Chemical Workforce: Diversity Models that Work" for the Chemical Science Roundtable, National Research Council, March 15-16, 2002

3. Chair and Co-organizer, Symposium on “Chemical Kinetics and the Environment,” for the American Chemical Society 210th National Meeting, Chicago, IL, August 20-25, 1995

EDITORIAL BOARDS

Member, Editorial Advisory Board, Journal of the American Chemical Society, Jan.1, 2014 – Dec, 31, 2017

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Member, Editorial Advisory Board, Theoretical Chemistry Accounts, Jan.1, 2013 - present

Member, Editorial Advisory Board, Computational and Theoretical Chemistry, Jan.1, 2011 – present.

Member, Editorial Advisory Board, Journal of Physical Chemistry, Jan.1, 2008 – Dec, 31, 2012.

Member, Editorial Advisory Board, Journal of Molecular Structure-Theochem, July 1, 2004-June 30, 2010

Atmospheric and Ocean Science Editor, Pure and Applied Geophysics, Jan. 6, 1998-Jan. 1, 2001

Member, Editorial Advisory Board, Advances in Environmental Research, July 1,1996 – present

Member, Editorial Advisory Board, Spectrochimica Acta, Part A, July 2, 1990 - present