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EDUCATION

08/1999 – 08/2004 ***Emory University***, Atlanta, GA, U.S.A., **Ph.D.** in Chemistry (Physical/Theoretical)

Thesis Title: *Full-dimensional quantum studies of the energetics and dynamics of H_3O^+, $H_3O_2^-$ and $H_5O_2^+$.*

Thesis Advisor : Professor Joel M. Bowman

09/1997 – 06/1999 ***Institute of Chemistry, CAS***, Beijing, P. R. China, **M.S. (*Not Completed*)**

09/1992 – 07/1997 ***Fudan University***, Shanghai, P. R. China, **B.S.** in Applied Chemistry (II)

RESEARCH INTEREST

Computational Molecular Spectroscopy & Dynamics for Astronomical Molecules: Theory and Applications.

PROFESSIONAL EXPERIENCE AND EMPLOYMENT HISTORY

06/2009 – present **SETI** (Search for Extra-Terrestrial Intelligence) Institute, Research Scientist

06/2006 – 05/2009 NASA Postdoctoral Fellow, NASA Ames Research Center (Advisor: Dr. Timothy J. Lee)

09/2004 – 12/2005 Post-doctoral Research Fellow, Emory University (Advisor: Professor Joel M. Bowman)

Member of ACS, AGU, AAS, and AAAS

Reviewer for *J.Chem.Phys., J.Phys.Chem. A, Mol. Phys., JQSRT, PCCP, and Advances in Space Research*

Co-Guest Editor for a special issue of "*Advances in Physical Chemistry*" entitled *Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy*, February, 2012

SCI PUBLICATION & CITATIONS (*2001-2014*) (ISI/Web of Science, 09/2014)

Total SCI publications: [60 Articles/Letters/Review/Proceedings +12 conferences + 1 dissertation]

60 Articles/Letter/Review have1726 citations, H-index = 25

SCIENTIFIC PRESENTATIONS AND TALKS

1. 248th ACS National Meeting, San Francisco, USA (Aug.10-14, 2014).
2. First Workshop on Experimental Laboratory Astrophysics, Kauai, HI, USA (Feb.25-27, 2013)
3. 44th–46th American Geophysical Union (AGU) Fall meeting, San Francisco, USA (2011-2013)
4. International Astronomical Union General Assembly XXVIII, SpS16 and S292, Beijing, China (2012).
5. 67th International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (2012).
6. Astrobiology Science Conference 2012, Atlanta, GA, USA (2012).
7. 65th International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (2010).
8. 59th Annual Conference of The Western Spectroscopy Association, Pacific Grove, CA, USA (2010)
9. 64th International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (2009).
10. 227th -239th ACS National Meeting, USA (2004-2009).
11. Advanced Workshop on Theoretical and Computational Methods for Molecular Spectroscopy and Collisions: Application to Astrophysical and Atmospheric Relevant Systems, Granada, Spain (2009).
12. Invited talks at Sichuan Univ., Suzhou Univ., & Dalian Institute of Chemical Physics (CAS), China (2009).
13. WATOC 2008, Sydney, Australia (2008).
14. Gordon Conference on Molecular Energy Transfer 2005, Santa Babara, CA, USA (2005).
15. CDMC 2003, Lake Tahoe, CA, USA (2003).
16. SERMACS, USA (2003-2005).

List of Peer-reviewed SCI Articles/Letters/Reviews/Proceedings (*2001-2014*)

1. **X. Huang**, R. R. Gamache, R. S. Freedman, D. W. Schwenke, T. J. Lee: *Reliable infrared line lists for 13 CO_2 isotopologues up to E'=18,000 cm^{-1} and 1500 K, with line shape parameters* J. Quant. Spectrosc. Radiat. Trans., **147**, 134-144 (*2014*). DOI: 10.1016/j.jqsrt.2014.05.015
2. R. C. Fortenberry, **X. Huang**, T. D. Crawford, and T. J. Lee: *Quartic Force Field Rovibrational Analysis of Protonated Acetylene, $C_2H_3^+$, and Its Isotopologues* J. Phys. Chem. A **118**, 7034-7043 (*2014*). DOI: 10.1021/jp506441g
3. L.-H. Xu, R. M. Lees, J. T. Hougen, J. M. Bowman, **X. Huang**, and S. Carter: *Comparison of independently calculated ab initio normal-mode displacements for the three C-H stretching vibrations of methanol along the internal rotation path*, J. Mol.

Spectrosc. **299**, 11-16 (*2014*). DOI: 10.1016/j.jms.2014.02.007

4. **X. Huang**, D. W. Schwenke, and T. J. Lee: *Highly accurate potential energy surface, dipole moment surface, rovibrational energy levels, and infrared line list for $^{32}S^{16}O_2$ up to 8000 cm^{-1}*, J. Chem. Phys. **140**, 114311 (*2014*). DOI: 10.1063/1.4868327
5. R. C. Fortenberry, **X. Huang**, D. W. Schwenke, and T. J. Lee: *Limited rotational and rovibrational line lists computed with highly accurate quartic force fields and ab initio dipole surfaces*, Spectrochim. Acta Part A, **119**, 76-83 (*2014*). DOI: 10.1016/j.saa.2013.03.092
6. X. Wang, **X. Huang**, J. M. Bowman, and T. J. Lee: *Anharmonic rovibrational calculations of singlet cyclic C-4 using a new ab initio potential and a quartic force field*, J. Chem. Phys., **139**, 224302 (*2013*). DOI: 10.1063/1.4837177
7. N. Inostroza, R. C. Fortenberry, **X. Huang**, and T. J. Lee: *Rovibrational Spectroscopic Constants and Fundamental Vibrational Frequencies for Isotopologues of Cyclic and Bent Singlet HC_2N Isomers*, Astrophys. J., **778**, 160, (*2013*). DOI:10.1088/0004-637X/778/2/160
8. **X. Huang**, R. S. Freedman, S. A. Tashkun, D. W. Schwenke, and T. J. Lee: *Semi-empirical $^{12}C^{16}O_2$ IR line lists for simulations up to 1500 K and 20,000 cm^{-1}*, J. Quant. Spectrosc. Radiat. Trans., **130**, 134-146 (*2013*). DOI:10.1016/j.jqsrt.2013.05.018
9. **X. Huang**, R. C. Fortenberry, and T. J. Lee: *Protonated nitrous oxide, $NNOH^+$: Fundamental vibrational frequencies and spectroscopic constants from quartic force fields*, J. Chem. Phys., **139**, 084313 (*2013*), DOI: 10.1063/1.4819069
10. R. C. Fortenberry, **X. Huang**, T. D. Crawford, and T. J. Lee: *High-accuracy Quartic Force Field Calculations for the Spectroscopic Constants and Vibrational Frequencies of 1 $^1A'$ l-C_3H^-: A Possible Link to Lines Observed in the Horsehead Nebula Photodissociation Region*, Astrophys. J., **772**, 39, (*2013*). DOI: 10.1088/0004-637X/772/1/39
11. **X. Huang**, R. C. Fortenberry, and T. J. Lee: *Spectroscopic Constants and Vibrational Frequencies for l-C_3H^+ and Isotopologues from Highly Accurate Quartic Force Fields: The Detection of l-C_3H^+ in the Horsehead Nebula PDR Questioned*, Astrophys. J. Lett. **768**, L25, (*2013*). DOI: 10.1088/2041-8205/768/2/L25
12. R. C. Fortenberry, **X. Huang**, D. W. Schwenke, and T. J. Lee: *Limited Rotational and Rovibrational Line Lists Computed with Highly Accurate Quartic Force Fields and Ab Initio Dipole Surfaces*, Spectrochim. Acta Part A **119**, 76-83 (*2014*). DOI:10.1016/j.saa.2013.03.092
13. R. C. Fortenberry, **X. Huang**, A. Yachmenev, W. Thiel, and T. J. Lee: *On the Use of Quartic Force Fields in Variational Calculations*, Chem. Phys. Lett, **574**, 1-12, (*2013*). DOI:10.1016/j.cplett.2013.03.078
14. **X. Huang**, D. W. Schwenke, T. J. Lee, K. Sung, and L. R. Brown: *Quantum IR line list of NH_3 and isotopologues for ISM and dwarf studies*, Proceedings of the International Astronomical Union, vol. **8**, no. **S292**, pp. 248-248, pub. Cambridge University Press (*2012*).
15. **X. Huang**, R. C. Fortenberry, Y. Wang, J. S. Francisco, T. D. Crawford, J. M. Bowman, and T. J. Lee: *Dipole Surface and Infrared Intensities for the cis-and trans-HOCO and DOCO Radicals*, J. Phys. Chem. A, **117**, 6932 − 6939, (*2013*). DOI:10.1021/jp3102546
16. R. C. Fortenberry, **X. Huang**, T. D. Crawford, and T. J. Lee: *The 1 $^3A'$ HCN and 1 $^3A'$ HCO^+ Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields*, J. Phys. Chem. A, **117**, 9324 − 9330, (*2013*). DOI:10.1021/jp309243s
17. R.C. Fortenberry, **X. Huang**, J.S. Francisco, T.D. Crawford, and T.J. Lee : *Fundamental Vibrational Frequencies and Spectroscopic Constants of $HOCS^+$, $HSCO^+$, and Isotopologues via Quartic Force Fields*, J. Phys. Chem. A, **116**, 9582-9590, *2012*.
18. K. Sung, L.R. Brown, **X. Huang**, D.W. Schwenke, T.J. Lee, S.L. Coy, and K.K. Lehmann : *Extended Line Positions, Intensities, Empirical Lower State Energies and Quantum Assignments of NH_3 from 6300 to 7000 cm^{-1}*, J. Quant. Spectrosc. Radiat. Trans., **113**, 1066-1083, *2012*.
19. R.C. Fortenberry, **X. Huang**, J.S. Francisco, T.D. Crawford, and 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*.
20. **X. Huang**, D.W. Schwenke, and T.J. Lee : *An Isotopic-Independent Highly Accurate Potential Energy Surface for CO_2 Isotopologues and an Initial $^{12}C^{16}O_2$ Infrared Line List*, J. Chem. Phys., **136**, 124311, *2012*.
21. N. Inostroza, **X. Huang**, and T.J. Lee : *Accurate ab initio Quartic Force Fields of Cyclice and Bent HC_2N Isomers*, J. Chem. Phys., **135**, 244310, *2011*.
22. R.C. Fortenberry, **X. Huang**, J.S. Francisco, T.D. Crawford, and T.J. Lee : *Vibrational Fundamental Frequencies and Spectroscopic Constants from Quartic Force Fields for cis-HOCO: the Radical and the Anion*, J. Chem. Phys., **135**, 214303, *2011*.
23. R.C. Fortenberry, **X. Huang**, J.S. Francisco, T.D. Crawford, and T.J. Lee : *The trans-HOCO radical: Quartic Force Fields, Vibrational Frequencies, and Spectroscopic Constants*, J. Chem. Phys., **135**, 134301, *2011*.
24. **X. Huang**, and T.J. Lee : *Spectroscopic Constants for ^{13}C and Deuterium Isotopologues of Cyclic and Linear $C_3H_3^+$*, Astrophysical Journal **736**, 33, *2011*.
25. **X. Huang**, P.R. Taylor, and T.J. Lee : *Highly accurate quartic force fields, vibrational frequencies, and spectroscopic constants for cyclic and linear $C_3H_3^+$*, J. Phys. Chem. A **115**, 5005-5016, *2011*.

26. Y. Wang, **X. Huang**, B. C. Shepler, B. J. Braams, and J. M. Bowman : *Flexible, ab initio potential, and dipole moment surfaces for water: I. Tests and applications for clusters up to the 22-mer*, J. Chem. Phys. **134**, 094509, *2011*.
27. **X. Huang**, D. W. Schwenke, and T. J. Lee : *Rovibrational spectra of Ammonia. II. Detailed analysis, comparison, and prediction of spectroscopic assignments for $^{14}NH_3$, $^{15}NH_3$, and $^{14}ND_3$*, J. Chem. Phys. **134**, 044321, *2011*.
28. **X. Huang**, D. W. Schwenke, and T. J. Lee : *Rovibrational spectra of Ammonia. I. Unprecedented accuracy of a potential energy surface used with nonadiabatic corrections*, J. Chem. Phys. **134**, 044320, *2011*.
29. **X. Huang**, E. F. Valeev, and T. J. Lee : *Comparison of one-particle basis set extrapolation to explicitly correlated methods for the calculation of accurate quartic force fields, vibrational frequencies, and spectroscopic constants: Application to H_2O, N_2H^+, NO_2^+, and C_2H_2*, J. Chem. Phys. **133**, 244108, *2010*.
30. Y. Wang, J. M. Bowman, and **X. Huang** : (Communication) *Prediction of the rate constant of bimolecular hydrogen exchange in the water dimer using an ab initio potential energy surface*, J. Chem. Phys. **133**, 111103, *2010*.
31. J. M. Bowman, B. J. Braams, S. Carter, C. Chen, G. Czako, B. Fu, **X. Huang**, E. Kamachik, A. R. Sharma, B. C. Shepler, Y. Wang, and Z. Xie : *Ab-initio-based potential energy surfaces for complex molecules and molecular complexes*, J. Phys. Chem. Lett. **1**, 1866-1874, *2010*.
32. **X. Huang**, and T. J. Lee : *An approach to include the effects of diffuse functions inpotential energy surface calculations*, J. Phys. Chem. A **113**, 11954-11962, *2009*.
33. **X. Huang**, and T. J. Lee : *Accurate ab initio quartic force fields for NH_2^- and CCH^- and rovibrational spectroscopic constants for their isotopologues*, J. Chem. Phys. **131**, 104301, *2009*.
34. T. J. Lee, **X. Huang**, and C. E. Dateo : *The effect of approximating some molecular integrals in coupled-cluster calculations: fundamental frequencies and rovibrational spectroscopic constants for isotopologues of cyclopropenylidene*, Mol. Phys. **107**, 1139-1152, *2009*.
35. **X. Huang**, D. W. Schwenke, and T. J. Lee : *An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH_3*, J. Chem. Phys. **129**, 214304, *2008*.
36. **X. Huang**, and T. J. Lee : *A procedure for computing accurate ab initio quartic force fields: Application to HO_2^+ and H_2O*, J. Chem. Phys. **129**, 044312, *2008*.
37. **X. Huang**, B. J. Braams, J. M. Bowman, R. E. A. Kelly, J. Tennyson, G. C. Groenenboom, and Ad van der Avoird : *New ab initio potential energy surface and vibrational-rotation-tunneling levels of $(H_2O)_2$ and $(D_2O)_2$*, J. Chem. Phys. **128**, 034312, *2008*.
38. **X. Huang**, S. Habershon, and J. M. Bowman : *Comparison of quantum, classical, and ring-polymer molecular dynamics infra-red spectra of $Cl^-\cdot(H_2O)$ and $H^+\cdot(H_2O)_2$*, Chem. Phys. Lett. **450**, 253-257, *2007.*
39. J. M. Bowman, **X. Huang**, N. C. Handy, and S. Carter : *Vibrational levels of methanol calculated by the reaction path version of MULTIMODE, using an ab initio, full-dimensional potential,* J. Phys. Chem. A, **111**, 7317-7321, *2007*.
40. C. E. Hinkle, A. B. McCoy, **X. Huang**, and J. M. Bowman : *Comment on "Nature of the chemical bond in protonated methane"*, J. Phys. Chem. A. **111**, 2033-2034, *2007*.
41. J. Wu, **X. Huang**, S. Carter, and J. M. Bowman : *Tests of MULTIMODE calculations of rovibrational energies of CH_4*, Chem. Phys. Lett. **426**, 285-289, *2007*.
42. **X. Huang**, L. M. Johnson, J. M. Bowman, and A. B. McCoy : *Deuteration effects on the structure and Infrared spectrum of CH_5^+*, J. Am. Chem. Soc. **128**, 3478-3479, *2006*.
43. **X. Huang**, A. B. McCoy, J. M. Bowman, L. M. Johnson, C. Savage, F. Dong, and D. J. Nesbitt : *Quantum deconstruction of the Infrared spectrum of CH_5^+*, Science **311**, 60-63, *2006*.
44. J. M. Bowman, **X. Huang**, L. B. Harding, and S. Carter : *The determination of molecular properties from MULTIMODE with an application to the calculation of Franck-Condon factors for photoionization of CF_3 to CF_3^+*, Mol. Phys. **104**, 33-45, *2006*.
45. **X. Huang**, B. J. Braams, and J. M. Bowman : *Ab initio potential energy and dipole moment surfaces of $(H_2O)_2$*, J. Phys. Chem. A. **110**, 445-451, *2006*.
46. A. B. McCoy, **X. Huang**, S. Carter, and J. M. Bowman : *Quantum studies of the vibrations in $H_3O_2^-$ and $D_3O_2^-$*, J. Chem. Phys. **123**, 064317, *2005*.
47. **X. Huang**, B. J. Braams, and J. M. Bowman : *Ab initio potential energy and dipole moment surfaces for $H_5O_2^+$*, J. Chem. Phys., **122**, 044308, *2005*.
48. N. I. Hammer, E. G. Diken, J. R. Roscioli, M. A. Johnson, E. M. Myshakin, K. D. Jordan, A. B. McCoy, **X. Huang**, J. M. Bowman, and S. Carter : *The vibrational predissociation spectra of the $H_5O_2^+\cdot RG_n(RG=Ar,Ne)$ clusters: Correlation of the solvent perturbations in the free OH and shared proton transitions of the Zundel ion*, J. Chem. Phys. **122**, 244301, *2005*.
49. A. B. McCoy, **X. Huang**, S. Carter, M. Y. Landeweer, and J. M. Bowman : *Full-dimensional vibrational calculations for $H_5O_2^+$ using an ab initio potential energy surface*, J. Chem. Phys. **122**, 061101, *2005*.
50. E. G. Diken, J. M. Headrick, J. R. Roscioli, J. C. Bopp, M. A. Johnson, A. B. McCoy, **X. Huang**, S. Carter, and J. M. Bowman : *Argon predissociation spectroscopy of the $OH^-\cdot H_2O$ and $Cl^-\cdot H_2O$ complexes in the 1000-1900 cm^{-1} region: Intramolecular bending transitions and the search for the shared-proton fundamental in the hydroxide monohydrate*, J. Phys. Chem. A **109**,

571-575, *2005*.

51. A. B. McCoy, B. J. Braams, A. Brown, **X. Huang**, Z. Jin, and J. M. Bowman : *Ab initio diffusion Monte Carlo calculations of the quantum behavior of CH_5^+ in full dimensionality*, J. Chem. Phys. **108**, 4991-4994, *2004*.
52. A. L. Kaledin, **X. Huang**, and J. M. Bowman : *Comparison of classical, new corrected-classical, and semiclassical IR spectra of non-rotating H_2O with quantum calculations*, Chem. Phys. Lett. **384**, 80-85, *2004*.
53. **X. Huang**, B. J. Braams, S. Carter, and J. M. Bowman : *Quantum calculations of vibrational energies of $H_3O_2^-$ on an ab initio potential*, J. Am. Chem. Soc., **126**, 5042–5043, *2004*.
54. **X. Huang**; H. M. Cho; S. Carter; L. Ojamäe; J. M. Bowman; S. J. Singer : *Full dimensional calculations of vibrational energies of $H_5O_2^+$* , J. Phys. Chem. A, **107**, 7142–7151, *2003*.
55. J. Dai, Z. Bacic, **X. Huang**, S. Carter, and J. M. Bowman : *A theoretical study of vibrational mode coupling in $H_5O_2^+$*, J. Chem. Phys. **119**, 6571-6580, *2003*.
56. J. M. Bowman, S. Carter, and **X. Huang** : *MULTIMODE: a code to calculate rovibrational energies of polyatomic molecules*, Int. Rev. Phys. Chem. **22**, 533-549, *2003*.
57. **X. Huang**, S. Carter, and J. M. Bowman : *Ab initio potential energy surface and rovibrational energies of H_3O^+ and its isotopomers*, J. Chem. Phys. **118**, 5431-5441, *2003*.
58. **X. Huang**, S. Carter, and J. M. Bowman : *Ab initio potential energy surface and rovibrational energies of H_3O^+ and its isotopomers*, J. Phys. Chem. B **106**, 8182-8188, *2002*.
59. J. M. Bowman, **X. Huang**, and S. Carter : *Full dimensional calculations of vibrational energies of H_3O^+ and D_3O^+*, Spectrochim. Acta Part A **58**, 839-848, *2002*.
60. J. M. Bowman, D. Wang, **X. Huang**, F. Huarte-Larranaga, and U. Manthe : *The importance of an accurate CH_4 vibrational partition function in full dimensionality calculations of the $H+CH_4 \rightarrow H_2+CH_3$ reaction*, J. Chem. Phys. **114**, 9683-9684, *2001*.