

# Xinchuan Huang, Ph.D.

Research Scientist (Principal Investigator), SETI Institute, Mountain View, CA 94043  
MS 245-6; Room 107, Bldg 245; NASA Ames Research Center, Moffett Field, CA 94035  
Email: [Xinchuan.Huang-1@nasa.gov](mailto:Xinchuan.Huang-1@nasa.gov) Phone: 650-604-6264 (Office)

## **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<sub>3</sub>O<sup>+</sup>, H<sub>3</sub>O<sup>-</sup> and H<sub>5</sub>O<sub>2</sub><sup>+</sup>.*  
Thesis Advisor : Professor Joel M. Bowman

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

## **RESEARCH INTEREST**

Computational Molecular Spectroscopy, IR line lists for Astronomical & Atmospheric Molecules, Astrophysics

## **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.*, *ApJ*, *MNRAS*, *J.Phys.Chem.*, *Mol.Phys.*, *JQSRT*, *JMSpec*, *PCCP*, and *Adv.Space Res.*, etc.  
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

## **RECENT PROJECTS (2006 – 2018)**

Highly accurate IR line lists for HCN / HNC in studies of (exo-)planetary atmospheres, *NASA Grant 16-PDART\_2-0080, P.I.*  
for SO<sub>2</sub> Isotopologues, *ab initio* IR Lists for H<sub>2</sub>O<sup>+</sup>, H<sub>2</sub>Cl<sup>+</sup>, and NH<sub>4</sub><sup>+</sup>, *NASA Grant 12-APRA12-0107, Co-I*

for Methane and Isotopologues, *NASA Grant 13-PATM13-0012, Co-I*

for 13 CO<sub>2</sub> Isotopologues up to 18,000 cm<sup>-1</sup> and 1500K. *Venus Express SI Program, Co-I*

for <sup>14</sup>NH<sub>3</sub>, <sup>15</sup>NH<sub>3</sub>, and H<sub>3</sub>O<sup>+</sup> *NASA Grant 10-APRA10-0096, Co-I*

for <sup>32</sup>S<sup>16</sup>O<sub>2</sub> at 296K, up to 6000 cm<sup>-1</sup>, *NASA Grant 08-APRA08-0050, Co-I*

Accurate rovibrational spectroscopic constants and high quality *ab initio* quartic force field for HO<sub>2</sub><sup>+</sup>, NH<sub>2</sub><sup>-</sup>, CCH<sup>-</sup>, C<sub>3</sub>H<sub>3</sub><sup>+</sup>, C<sub>3</sub>H<sup>+</sup>, N<sub>2</sub>OH<sup>+</sup>, C<sub>2</sub>H<sub>2</sub>N<sup>+</sup>, etc..

Anharmonic IR analysis of Polycyclic Aromatic Hydrocarbons (PAH) and derivatives.

## **Recent Invited Talks**

254<sup>th</sup> ACS National Meeting, *Molecules in Space: Linking the Interstellar Medium to (Exo)-Planets* D.C., USA (08/2017)

Workshop on Astrophysical Opacities, Kalamazoo, MI, USA (08/2017)

Stars and Planets Seminar Series, Harvard-Smithsonian Center for Astrophysics, Boston, MA, USA (03/2017)

Workshop on Mass-Independent Fractionation of Sulfur Isotopes: Possible Molecular Origins, Telluride, CO, USA (2016)

## **SCI Publications & Citations (2001-2018)**

Total SCI publications: **74** Articles/Letters/Reviews, **29** 1<sup>st</sup>-author papers.

71 Articles/Letter/Review have **3048** citations from >**1500** articles, **H-index = 35** (*ISI/Web of Science*, 04/2018)

## **Full List of Peer-reviewed SCI Articles/Letters/Reviews and Conference Proceedings (2001-2018)**

1. N. Rangwala, S.W.J. Colgan, R.L. Gal, K. Acharyya, **X. Huang**, T.J. Lee, E. Herbst, C. DeWitt, M. Richter, A. Boogert, M. McKelvey: “*High Spectral Resolution SOFIA/EXES Observations of C<sub>2</sub>H<sub>2</sub> toward Orion Irc2*” *ApJ* **856**, 9 (2018), [online](#)
2. E. Maltseva, C.J. Mackie, A. Cadian, A. Petrignani, **X. Huang**, T.J. Lee, A.G.G.M. Tielens, J. Oomens, and W.Jan Buma: “*High-resolution IR absorption spectroscopy of PAH in the 3 um region: role of hydrogenation and alkylation*”, *A&A* **610**, A65 (2018), [online](#)
3. C.J. Mackie, A. Cadian, **X. Huang**, E. Maltseva, A. Petrignani, J. Oomens, W.J. Buma, T.J. Lee and A.G.G.M. Tielens: *The anharmonic quartic force field infrared spectra of hydrogenated and methylated PAHs*”, *PCCP* **20**, 1189-1197 (2018), [online pdf](#)
4. **X. Huang**, D.W. Schwenke, R.S. Freedman, and T.J. Lee: *Ames-2016 line lists for 13 isotopologues of CO<sub>2</sub>: Updates, consistency, and remaining issues*. *JQSRT*, **203**, 224-241 (2017), [Open access](#)
5. R.R. Gamache, C. Roller, E. Lopes, I.E. Gordon, L.S Rothman, O.L Polyansky, N.F. Zobov, A.A. Kyuberis, J. Tennyson, S.N. Yurchenko, A.G. Csaszar, T. Furtenbacher, **X. Huang**, D.W. Schwenke, T.J. Lee, B.J. Drouin, S.A. Tashkun, V.I. Perevalov, R.V. Kochanov: *Total internal partition sums for 166 isotopologues of 51 molecules important in planetary atmospheres: Application to HITRAN2016 and beyond* *J.Quant.Spectrosc.Ra.* **203**, 70-87 (2017) [online](#)

6. R.C. Fortenberry, T.J. Lee, **X. Huang** : *Towards completing the cyclopropenylidene cycle: rovibrational analysis of cyclic  $N_3^+$ , CNN, HCNN<sup>+</sup>, and CNC*, *Phys.Chem.Chem.Phys.* **19**, 22860-22869 (2017) [online](#)
7. **X. Huang**, D.W. Schwenke, T.J. Lee: *Ames  $^{16}O^{32}S^{18}O$  line list for high-resolution experimental IR analysis*, *J.Mol.Spectrosc.* **330**, 101-111 (2016), [online](#)
8. E. Maltseva, A. Petrignani, A. Candian, C.J. Mackie, **X. Huang**, T.J. Lee, A.G.G.M. Tielens, J. Oomens, W.J. Buma: *High-resolution IR absorption Spectroscopy of Polycyclic Aromatic Hydrocarbons in the 3  $\mu m$  region: role of Periphery*. *ApJ*, **831**(1), 58 (2016) [pdf](#)
9. C.J. Mackie, A. Candian, **X. Huang**, E. Maltseva, A. Petrignani, J. Oomens, W.J. Buma, T.J. Lee, A.G.G.M. Tielens: *The anharmonic force field infrared spectra of five non-linear polycyclic aromatic hydrocarbons: Benzanthracene, chrysene, phenathrene, pyrene, and triphenylene* *J.Chem.Phys.* **145**, 084313 (2016). [online](#)
10. D.S. Underwood, J. Tennyson, S.N. Yurchenko, **X. Huang**, D.W. Schwenke, T.J. Lee, S. Clausen, A. Fateev : *ExoMol molecular line lists – XIV. The rotation-vibration spectrum of hot SO<sub>2</sub>* *Mon.Not.R.Astron.Soc.* **459**, 3890 (2016). [online](#)
11. C.J. Mackie, A. Candian, **X. Huang**, E. Maltseva, A. Petrignani, J. Oomens, W.J. Buma, T.J. Lee, A.G.G.M. Tielens: *The anharmonic quartic force field infrared spectra of three polycyclic aromatic hydrocarbons: Naphthalene, Anthracene, and Tetracene* *J. Chem. Phys.* **143**, 224314 (2015). [online pdf](#)
12. E. Maltseva, A. Petrignani, A. Candian, C.J. Mackie, **X. Huang**, T.J. Lee, A.G.G.M. Tielens, J. Oomens, W.J. Buma : *High-resolution IR absorption spectroscopy of polycyclic aromatic hydrocarbons: the realm of anharmonicity* *Astrophys. J.* **814**(1), 23 (2015) [PDF](#)
13. C.J. Mackie, A. Candian, **X. Huang**, T.J. Lee, A.G.G.M Tielens : *Linear transformation of anharmonic molecular force constants between normal and Cartesian coordinates* *J.Chem.Phys.* **142**, 244107 (2015) [online](#)
14. **X. Huang**, D.W. Schwenke, and T.J. Lee: *Empirical Infrared line lists for five SO<sub>2</sub> isotopologues:  $^{32/33/34/36}SO_2$  and  $^{32}S^{18}O_2$*  *J.Mol.Spectrosc.* **311**, 19-24 (2015). [online](#)
15. R.C. Fortenberry, **X. Huang**, T.D. Crawford, T.J. Lee: *Quantum Chemical Rovibrational Data for the Interstellar Detection of c-C<sub>3</sub>H* *Astrophys. J.* **796**, 139 (2014). [online pdf](#)
16. **X. Huang**, R.R. Gamache, R.S. Freedman, D.W. Schwenke, T.J. Lee: *Reliable infrared line lists for 13 CO<sub>2</sub> isotopologues up to E'=18,000 cm<sup>-1</sup> and 1500 K, with line shape parameters* *J.Quant.Spectrosc.Ra.* **147**, 134-144 (2014). [online](#)
17. R.C. Fortenberry, **X. Huang**, T.D. Crawford, T.J. Lee : *Quartic Force Field Rovibrational Analysis of Protonated Acetylene, C<sub>2</sub>H<sub>3</sub><sup>+</sup>, and Its Isotopologues* *J.Phys.Chem.A* **118**, 7034 (2014) [online](#)
18. R.C. Fortenberry, **X. Huang**, M.C. McCarthy, T.D. Crawford, T.J. Lee : *Fundamental Vibrational Frequencies and Spectroscopic Constants of cis- and trans-HOCS, HSCO, and Isotopologues via Quartic Force Fields* *J.Phys.Chem.B* **118**, 6498-6510 (2014) [online](#)
19. L.-H. Xu, R.M. Lees, J.T. Hougen, J.M. Bowman, **X. Huang**, 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) [online](#)
20. **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<sup>-1</sup>*, *J. Chem. Phys.* **140**, 114311 (2014). [online](#)
21. 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). [online](#)
22. X. Wang, **X. Huang**, J.M. Bowman, T.J. Lee: *Anharmonic rovibrational calculations of singlet cyclic C<sub>4</sub> using a new ab initio potential and a quartic force field* *J.Chem.Phys.* **139**, 224302 (2013). [online](#)
23. 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<sub>2</sub>N Isomers*, *Astrophys. J.*, **778**, 160, (2013). [online pdf](#)
24. **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<sup>-1</sup>*, *J.Quant.Spectrosc.Ra.* **130**, 134-146 (2013). [online](#)
25. R. C. Fortenberry, **X. Huang**, T.D. Crawford, and T. J. Lee: *The 1  $^3A'$  HCN and 1  $^3A'$  HCO<sup>+</sup> Vibrational Frequencies and Spectroscopic Constants from Quartic Force Fields*, *J. Phys. Chem. A*, **117**, 9324-9330, (2013). [online](#)
26. **X. Huang**, R.C. Fortenberry, and T. J. Lee: *Protonated nitrous oxide, NNOH<sup>+</sup>: Fundamental vibrational frequencies and spectroscopic constants from quartic force fields*, *J. Chem. Phys.*, **139**, 084313 (2013). [online](#)
27. **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). [online](#)
28. 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<sub>3</sub>H: A Possible Link to Lines Observed in the Horsehead Nebula Photodissociation Region*, *Astrophys. J.*, **772**, 39, (2013). [online pdf](#)
29. 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). [online](#)
30. **X. Huang**, R.C. Fortenberry, and T.J. Lee: *Spectroscopic Constants and Vibrational Frequencies for l-C<sub>3</sub>H<sup>+</sup> and Isotopologues from Highly Accurate Quartic Force Fields: The Detection of l-C<sub>3</sub>H<sup>+</sup> in the Horsehead Nebula PDR Questioned*, *Astrophys. J. Lett.* **768**, L25, (2013). [online PDF](#)

31. R.C. Fortenberry, **X. Huang**, J.S. Francisco, T.D. Crawford, and T.J. Lee : *Fundamental Vibrational Frequencies and Spectroscopic Constants of HOCS<sup>+</sup>, HSCO<sup>+</sup>, and Isotopologues via Quartic Force Fields*, *J.Phys.Chem.A*, **116**, 9582-9590, 2012. [online](#)
32. 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<sub>3</sub> from 6300 to 7000 cm<sup>-1</sup>*, *J.Quant.Spectrosc.Ra.*, **113**, 1066-1083, 2012. [online](#)
33. 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<sup>+</sup> and DOCO<sup>+</sup>*, *J.Chem.Phys.*, **136**, 234309, 2012. [online](#)
34. **X. Huang**, D.W. Schwenke, and T.J. Lee : *An Isotopic-Independent Highly Accurate Potential Energy Surface for CO<sub>2</sub> Isotopologues and an Initial <sup>12</sup>C<sup>16</sup>O<sub>2</sub> Infrared Line List*, *J. Chem. Phys.*, **136**, 124311, 2012. [online](#)
35. N. Inostroza, **X. Huang**, and T.J. Lee : *Accurate ab initio Quartic Force Fields of Cyclic and Bent HC<sub>2</sub>N Isomers*, *J.Chem.Phys.*, **135**, 244310, 2011. [online](#)
36. 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. [online](#)
37. 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. [online](#)
38. **X. Huang**, and T.J. Lee : *Spectroscopic Constants for <sup>13</sup>C and Deuterium Isotopologues of Cyclic and Linear C<sub>3</sub>H<sub>3</sub><sup>+</sup>*, *Astrophys. J.* **736**, 33, 2011. [online PDF](#)
39. **X. Huang**, P.R. Taylor, and T.J. Lee : *Highly accurate quartic force fields, vibrational frequencies, and spectroscopic constants for cyclic and linear C<sub>3</sub>H<sub>3</sub><sup>+</sup>*, *J. Phys. Chem. A* **115**, 5005-5016, 2011. [online](#)
40. 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. [online](#)
41. **X. Huang**, D.W. Schwenke, and T.J. Lee : *Rovibrational spectra of Ammonia. II. Detailed analysis, comparison, and prediction of spectroscopic assignments for <sup>14</sup>NH<sub>3</sub>, <sup>15</sup>NH<sub>3</sub>, and <sup>14</sup>ND<sub>3</sub>*, *J. Chem. Phys.* **134**, 044321, 2011. [online](#)
42. **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. [online](#)
43. **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<sub>2</sub>O, N<sub>2</sub>H<sup>+</sup>, NO<sub>2</sub><sup>+</sup>, and C<sub>2</sub>H<sub>2</sub>*, *J. Chem. Phys.* **133**, 244108, 2010. [online](#)
44. 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. [pdf \(open access\)](#)
45. 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. [online](#)
46. **X. Huang**, and T.J. Lee : *An approach to include the effects of diffuse functions in potential energy surface calculations*, *J. Phys. Chem. A* **113**, 11954-11962, 2009. [online](#)
47. **X. Huang**, and T.J. Lee : *Accurate ab initio quartic force fields for NH<sub>2</sub><sup>-</sup> and CCH<sup>-</sup> and rovibrational spectroscopic constants for their isotopologues*, *J. Chem. Phys.* **131**, 104301, 2009. [online](#)
48. 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. [online](#)
49. **X. Huang**, D.W. Schwenke, and T.J. Lee : *An accurate global potential energy surface, dipole moment surface, and rovibrational frequencies for NH<sub>3</sub>*, *J. Chem. Phys.* **129**, 214304, 2008. [online](#)
50. **X. Huang**, and T.J. Lee : *A procedure for computing accurate ab initio quartic force fields: Application to HO<sub>2</sub><sup>+</sup> and H<sub>2</sub>O*, *J. Chem. Phys.* **129**, 044312, 2008. [online](#)
51. **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<sub>2</sub>O)<sub>2</sub> and (D<sub>2</sub>O)<sub>2</sub>*, *J. Chem. Phys.* **128**, 034312, 2008. [online](#)
52. **X. Huang**, S. Habershon, and J.M. Bowman : *Comparison of quantum, classical, and ring-polymer molecular dynamics infra-red spectra of Cl<sup>-</sup>(H<sub>2</sub>O) and H<sup>+</sup>(H<sub>2</sub>O)<sub>2</sub>*, *Chem. Phys. Lett.* **450**, 253-257, 2007. [online](#)
53. 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. [online](#)
54. 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. [online](#)
55. J. Wu, **X. Huang**, S. Carter, and J.M. Bowman : *Tests of MULTIMODE calculations of rovibrational energies of CH<sub>4</sub>*, *Chem. Phys. Lett.* **426**, 285-289, 2007. [online](#)
56. **X. Huang**, L.M. Johnson, J.M. Bowman, and A.B. McCoy : *Deuteration effects on the structure and Infrared spectrum of CH<sub>5</sub><sup>+</sup>*, *J. Am. Chem. Soc.* **128**, 3478-3479, 2006. [online](#)

57. **X. Huang**, B.J. Braams, and J.M. Bowman : *Ab initio potential energy and dipole moment surfaces of (H<sub>2</sub>O)<sub>2</sub>*, *J. Phys. Chem. A.* **110**, 445-451, 2006. [online](#)
58. 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<sub>3</sub> to CF<sub>3</sub><sup>+</sup>*, *Mol. Phys.* **104**, 33-45, 2006. [online](#)
59. **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<sub>5</sub><sup>+</sup>*, *Science* **311**, 60-63, 2006. [online](#)
60. A.B. McCoy, **X. Huang**, S. Carter, and J.M. Bowman : *Quantum studies of the vibrations in H<sub>3</sub>O<sub>2</sub><sup>-</sup> and D<sub>3</sub>O<sub>2</sub><sup>-</sup>*, *J. Chem. Phys.* **123**, 064317, 2005. [online](#)
61. 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<sub>5</sub>O<sub>2</sub><sup>+</sup>·RG<sub>n</sub>(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. [online](#)
62. A.B. McCoy, **X. Huang**, S. Carter, M.Y. Landeweer, and J.M. Bowman : *Full-dimensional vibrational calculations for H<sub>5</sub>O<sub>2</sub><sup>+</sup> using an ab initio potential energy surface*, *J. Chem. Phys.* **122**, 061101, 2005. [online](#)
63. 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·H<sub>2</sub>O and Cl·H<sub>2</sub>O complexes in the 1000-1900 cm<sup>-1</sup> region: Intramolecular bending transitions and the search for the shared-proton fundamental in the hydroxide monohydrate*, *J. Phys. Chem. A* **109**, 571-575, 2005. [online](#)
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65. 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<sub>5</sub><sup>+</sup> in full dimensionality*, *J. Chem. Phys.* **108**, 4991-4994, 2004. [online](#)
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67. A.L. Kaledin, **X. Huang**, and J.M. Bowman : *Comparison of classical, new corrected-classical, and semiclassical IR spectra of non-rotating H<sub>2</sub>O with quantum calculations*, *Chem. Phys. Lett.* **384**, 80-85, 2004. [online](#)
68. J. Dai, Z. Bacic, **X. Huang**, S. Carter, and J.M. Bowman : *A theoretical study of vibrational mode coupling in H<sub>5</sub>O<sub>2</sub><sup>+</sup>*, *J. Chem. Phys.* **119**, 6571-6580, 2003. [online](#)
69. **X. Huang**; H.M. Cho; S. Carter; L. Ojamäe; J.M. Bowman; S.J. Singer : *Full dimensional calculations of vibrational energies of H<sub>5</sub>O<sub>2</sub><sup>+</sup>*, *J. Phys. Chem. A* **107**, 7142-7151, 2003. [online](#)
70. 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. [online](#)
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## Previous Scientific Presentations

- 8<sup>th</sup> Molecular Quantum Mechanics, Uppsala, Sweden (2016)
- 44<sup>th</sup>-48<sup>th</sup> American Geophysical Union (AGU) Fall meeting, San Francisco, USA (2011-2015).
- International Astronomical Union General Assembly XXIX, FM12, Honolulu , USA (2015).
- 70<sup>th</sup> International Symposium on Molecular Spectroscopy, UIUC, Illinois, USA (2015).
- First Workshop on Experimental Laboratory Astrophysics, Kauai, HI, USA (2013)
- Workshop on Molecular Spectroscopy in the Era of Far-IR Astronomy, Atlanta, GA, USA (2012)
- International Astronomical Union General Assembly XXVIII, SpS16 and S292, Beijing, China (2012).
- Astrobiology Science Conference 2012, Atlanta, GA, USA (2012).
- 64<sup>th</sup>/65<sup>th</sup>/67<sup>th</sup> International Symposium on Molecular Spectroscopy, Columbus, Ohio, USA (2009-2010,2012).
- Molecular Quantum Mechanics 2010, Berkeley, CA, USA (2010)
- 59<sup>th</sup> Annual Conference of the Western Spectroscopy Association, Pacific Grove, CA, USA (2010)
- 227<sup>th</sup> -239<sup>th</sup> ACS National Meeting, USA (2004-2009).
- Advanced Workshop on Theoretical and Computational Methods for Molecular Spectroscopy and Collisions: Application to Astrophysical and Atmospheric Relevant Systems, Granada, Spain (2009).
- Invited talks at Sichuan Univ., Suzhou Univ., & Dalian Institute of Chemical Physics (CAS), China (2009).
- The 2008 World Congress of WATOC, Sydney, Australia (2008).
- Gordon Conference on Molecular Energy Transfer 2005, Santa Barbara, CA, USA (2005).
- Conference on Dynamics of Molecular Collisions 2003, Lake Tahoe, CA, USA (2003).
- SERMACS, USA (2003-2005).