QI YU

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RESEARCH INTEREST

Electronic Structure Theory, Vibrational Spectroscopy, Potential Energy Surface, Machine Learning, Ion-water interaction

EDUCATION

Emory University Aug. 2014 - Aug. 2019
Ph.D in Chemistry *Advisor: Prof. Joel M. Bowman*

University of Science and Technology of China (USTC) Sep. 2010 - Jul. 2014
B.S. in Chemical Physics *Advisor: Prof. Shanxi Tian*

PROFESSIONAL EXPERIENCE

Yale University Oct. 2019 - present
Postdoctoral Associate *Advisor: Prof. Sharon Hammes-Schiffer*

Dalian Institute of Chemical Physics, Chinese Academy of Science May. 2013 - Aug. 2013
Visiting Student *Advsor: Prof. Donghui Zhang*

HONORS AND AWARDS

Chinese Outstanding Student Abroad Award	2019
Quayle Student Achievement Award from Emory	2018
Outstanding Student Scholarship from USTC	2013
National Scholarship for Encouragement from USTC	2012
National Scholarship from USTC	2011
Outstanding Freshman Scholarship from USTC	2010

PUBLICATIONS (TOTAL = 25, H-INDEX = 15, CITATION= 554)

*Corresponding author

1. **Q. Yu**, P. E. Schneider and S. Hammes-Schiffer . "Transition States and Reaction Path using the Nuclear-electronic Orbital Multistate Density Functional theory ." ***In preparation***, **2021**.
2. Z. Tao, **Q. Yu**, S. Roy and S. Hammes-Schiffer . "Direct Dynamics with Nuclear-Electronic Orbital Density Functional Theory ." ***Acc. Chem. Res.***, under review. **2021**
3. B. Dereka, **Q. Yu**, N. H.C. Lews, W. B. Carpenter, J. M. Bowman and A. Tokmakoff . "Crossover from Hydrogen to Chemical Bonding ." ***Science***, 371,160-164, **2021**.[pdf]
4. **Q. Yu** and S. Hammes-Schiffer. "Nuclear-Electronic Orbital Multistate Density Functional Theory." ***J. Phys. Chem. Lett.***, 11, 10106 **2020**.[pdf]

5. W. B. Carpenter, **Q. Yu**, J. H. Hack, B. Dereka, J. M. Bowman and A. Tokmakoff . "Decoding the 2D IR Spectrum of the Aqueous Proton with High-Level VSCF/VCI Calculations ." ***J. Chem. Phys***, 153, 124506, **2020**.[pdf]

6. **Q. Yu**, F. Pavosevic and S. Hammes-Schiffer. "Developing of nuclear basis sets for multicomponent quantum chemistry methods." ***J. Chem. Phys.***, 152, 244123, **2020**. [pdf]

7. **Q. Yu***, J. M. Bowman. "Tracking Hydronium/Water Stretches in Magic $H_3O^+(H_2O)_{20}$ Clusters through High-level Quantum VSCF/VCI Calculations." ***J. Phys. Chem. A***, 124, 1167-1175, **2020**. [pdf]

8. **Q. Yu***, W. B. Carpenter, N. H.C. Lews, A. Tokmakoff and J. M. Bowman. "High-Level VSCF/VCI Calculations Decode the Vibrational Spectra of Aqueous Proton." ***J. Phys. Chem. B***, 123(33), 7214-7224, **2019**. [pdf]

9. C. H. Duong, N. Yang, R. J. DiRisio, **Q. Yu**, M. A. Johnson, A. B. McCoy and J. M. Bowman. "Disentangling the Complex Vibrational Mechanics of the Protonated Water Trimer by Rational Control of Its Hydrogen Bonds." ***J. Phys. Chem. A***, 123(37), 7965-7972, **2019**. [pdf]

10. **Q. Yu** and J. M. Bowman. "Classical, Thermostated Ring Polymer, and Quantum VSCF/VCI Calculations of IR Spectra of $H_7O_3^+$ and $H_9O_4^+$ (Eigen) and Comparison with Experiment." ***J. Phys. Chem. A***, 123(7), 1399-1409, **2019**.[pdf]

11. P. L. Houston, B. L.V. Hoozen, C. Qu, **Q. Yu** and J. M. Bowman. "Teaching Vibrational Spectra to Assign Themselves." ***Faraday Discussions***, 212, 65-82, **2018**.[pdf]

12. T. Q. Bui, P. B. Changala, B. J. Bjork, **Q. Yu**, Y. Wang, J. F. Stanton, J. M. Bowman and J. Ye. "Spectral Analyses of Trans- and Cis-DOCO Transients via Comb Spectroscopy." ***Molecular Physics***, 116, 3710-3717, **2018**.[pdf]

13. C. H. Duong, N. Yang, P. J. Kelleher, R. J. DiRisio, **Q. Yu**, B. V. Henderson, M. A. Johnson, A. B. McCoy, J. M. Bowman and K. D. Jordan. "Tag-Free and Isotopomer-Selective Vibrational Spectroscopy of the Cryogenically Cooled $H_9O_4^+$ Cation with Two-Color, IRIR Double-Resonance Photoexcitation: Isolating the Spectral Signature of a Single OH Group in the Hydronium Ion Core." ***J. Phys. Chem. A***, 122(48), 9275-9284, **2018**.[pdf]

14. **Q. Yu**, J. P. Heindel, J. M. Bowman and S. S. Xantheas. "Benchmark Electronic Structure Calculations for $H_3O^+(H_2O)$n, n = 0–5, Clusters and Tests of an Existing 1,2,3-Body Potential Energy Surface with a New 4-Body Correction." ***J. Chem. Theory Comput.***, 14(9), 4553-4566, **2018**.[pdf]

15. C. Qu, **Q. Yu**, B. V. Hoozen, J. M. Bowman and R. Vargas-Hernandez. "Assessing Gaussian Process Regression and Permutationally Invariant Polynomial Approaches To Represent High-Dimensional Potential Energy Surfaces." ***J. Chem. Theory Comput.***, 14(7), 3381-3396, **2018**.[pdf]

16. C. Qu, **Q. Yu** and J. M. Bowman. "Permutationally Invariant Potential Energy Surfaces." ***Annu. Rev. Phys. Chem.***, 69, 6.1-6.25, **2018**.[pdf]

17. T. K. Esser, **Q. Yu**, H. Knorke, W. Schöllkopf, C. Qu, K. R. Asmis, J. M. Bowman and M. Kaledin. "Deconstructing Prominent Bands in the Terahertz Spectra of $H_7O_3^+$ and $H_9O_4^+$: Intermolecular Modes in Eigen Clusters." ***J. Phys. Chem. Lett.***, 9(4), 798-803, **2018**.[pdf]

18. **Q. Yu** and J. M. Bowman. "High-Level Quantum Calculations of the IR Spectra of the Eigen, Zundel, and Ring Isomers of $H^+(H_2O)_4$ Find a Single Match to Experiment." ***J. Am. Chem. Soc.***, 139(32), 10984-10987, **2017**.[pdf]

19. C. H. Duong, O. Gorlova, **Q. Yu**, N. Yang, P. J. Kelleher, M. A. Johnson, A. B. McCoy and J. M. Bowman. "Disentangling the Complex Vibrational Spectrum of the Protonated Water Trimer, $H^+(H_2O)_3$, with Two-Color IR-IR Photodissociation of the Bare Ion and Anharmonic VSCF/VCI Theory." ***J. Phys. Chem. Lett.***, 8(16), 3782-3789, **2017**.[pdf]

20. **Q. Yu** and J. M. Bowman. "VSCF/VCI Vibrational Spectroscopy of $H_7O_3^+$ and $H_9O_4^+$ using High-level, Many-

body Potential Energy Surface and Dipole Moment Surfaces." ***J. Chem. Phys.***, 146(12), 121102, **2017**.[pdf]

21. **Q. Yu** and J. M. Bowman. "How the Zundel ($H_5O_2^+$) Potential Can Be Used to Predict the Proton Stretch and Bend Frequencies of Larger Protonated Water Clusters." ***J. Phys. Chem. Lett.***, 7(24), 5259-5265, **2016**.[pdf]
22. **Q. Yu** and J. M. Bowman. "Ab Initio Potential for $H_3O^+ \rightarrow H^+ + H_2O$: A Step to a Many-Body Representation of the Hydrated Proton?." ***J. Chem. Theory Comput.***, 12(11), 5284-5292, **2016**.[pdf]
23. **Q. Yu** and J. M. Bowman. "Vibrational Second-order Perturbation Theory (VPT2) using Local Monomer Normal Modes." ***Mol. Phys.***, 113(24), 3964-4971, **2015**.[pdf]
24. **Q. Yu**, J. M. Bowman, R. C. Fortenberry, J. S. Mancini, T. J. Lee, T. D. Crawford, W. Klemperer and J. S. Francisco. "Structure, Anharmonic Vibrational Frequencies, and Intensities of $NNHNN^+$." ***J. Phys. Chem. A***, 119(47), 11623-11631, **2015**.[pdf]
25. R. C. Fortenberry, **Q. Yu**, J. S. Mancini, J. M. Bowman, T. J. Lee, T. D. Crawford, W. Klemperer and J. S. Francisco. "Spectroscopic Consequences of Proton Delocalization in $OCHCO^+$." ***J. Chem. Phys.***, 143(7), 071102, **2015**.[pdf]

ORAL TALKS

1. "MULTIMODE: A code to calculate rovibrational spectra of polyatomic molecules", *MolSSI Workshop on Rovibraional Molecular Spectroscopy*, Blacksburg, U.S., 2019.
2. "Quantum calculation of vibrational spectra of hydrated proton using many-body ab initio potential: from gas phase clusters to aqueous proton", *Spring ACS National Meeting*, Orlando, U.S., 2019.
3. "Benchmark electronic structure calculations for $H_3O^+(H_2O)$n,n=0-5 clusters and tests of a high-level many-body potential energy surface", *Atlanta Mini Symposium on Theoretical and Computational Chemistry*, Atlanta, U.S., 2018.

POSTER PRESENTATION

1. *Machine Learning in Science and Engineering*, Atlanta, GA, Jun. 2019.
2. *Gordon Research Conference: Molecular Interactions and Dynamics* , Boston, MA, Jul. 2018.
3. *Southeastern Theoretical Chemistry Association Metting*, University, MS, May 2017.
4. *Gordon Research Conference: Molecular Interactions and Dynamics* , Boston, MA, Jul. 2016.

TEACHING EXPERIENCE

Teaching Assistant — Spring 2016
Chem-332: Physical Chemistry II — *Emory University*

Teaching Assistant — Spring 2015
Chem-142: General Chemistry Lab — *Emory University*

Teaching Assistant — Fall 2014
Chem-141: General Chemistry Lab — *Emory University*

REFERENCES

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