

## WOLFGANG JAEGER

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### UNIVERSITY EDUCATION

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- 1985 - 1989 PhD Thesis in Physical Chemistry at the University of Kiel, Kiel, Germany:  
"Two-Dimensional Fourier Transform Spectroscopy in the Microwave Radio Frequency Range and Spectroscopic Studies of Methyl Thiazoles"; Minors: Astronomy, Organic Chemistry, Standing: "magna cum laude".
- 1984 - 1985 Diploma Thesis at the University of Kiel: "Microwave Spectroscopic Studies on 4-Methyl Isoxazole:  $^{14}\text{N}$  Nuclear Quadrupole Hyperfine Structure, Dipole Moment, and Barrier to Internal Rotation".
- 1977 - 1985 Studies in Chemistry, University of Kiel

### PROFESSIONAL POSITIONS

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- 2009 - 2010 Visiting Scientist, Fritz-Haber Institute of the MPS, Berlin, Germany
- 2003 - present Professor, Department of Chemistry, University of Alberta
- 2001 - 2003 Associate Professor, Department of Chemistry, University of Alberta
- 1995 - 2001 Assistant Professor, Department of Chemistry, University of Alberta
- 1995 (2 months) Visiting Scientist, I. Physical Institute, University of Cologne
- 1991 - 1995 Research Associate, Department of Chemistry, University of BC
- 1990 - 1991 Scientific Co-worker, Institute for Physical Chemistry, University of Kiel
- 1989 - 1990 Postdoctoral Fellow, Department of Chemistry, University of BC
- 1985 - 1989 Scientific Co-worker, Institute for Physical Chemistry, University of Kiel

### AWARDS

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- 2019 John C. Polanyi Award, Canadian Society for Chemistry
- 2018 Honoree of the *World Famous Scientist Lecture Series* Program, Hubei Province, China
- 2012 International Dr. Barbara Metz-Stark Prize
- 2011 Morino Lecture Award, Japan
- 2011 Renewal of Tier I Canada Research Chair in Cluster Science
- 2009 Humboldt Research Award, Humboldt Foundation, Germany
- 2008 - 2011 Discovery Accelerator Supplement, NSERC
- 2008 Fellow of the Royal Society of Canada
- 2004 - 2018 Canada Research Chair in Cluster Science (Tier I, Senior Chair)
- 2004 Canada Foundation for Innovation, CRC Award
- 2002 - 2004 Natural Sciences and Engineering Research Council Steacie Fellowship
- 2003 Noranda Award, Canadian Society for Chemistry
- 2002 Canada Foundation for Innovation, Career Award
- 2002 Canada Foundation for Innovation, Innovation Fund Award
- 2001 Faculty of Science Research Award, University of Alberta

## SCIENTIFIC COMMITTEES / FUNCTIONS (2012 – 2022)

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- 2022 7<sup>th</sup> Vibrational Optical Activity Conference, Canada, Co-Organizer
- 2022 Canadian Chemistry Conference and Exhibition, Co-Organizer, Symposium: "Advances in Molecular Spectroscopy - Experiment and Theory"
- 2022 XX<sup>th</sup> International Workshop on Quantum Molecular Tunneling Systems, Canada, Organizer
- 2020 Pacificchem 2020, Co-organizer, Symposium: "Terahertz imaging, spectroscopy and nanosensors: current applications and future direction"
- 2018 101<sup>st</sup> Canadian Society for Chemistry Conference, Co-Organizer, Symposium: "Spectroscopic Tools for Atmospheric Chemistry"
- 2016 - 2019 NSERC-Chemistry Liaison Committee
- 2016 99<sup>th</sup> Canadian Society for Chemistry Conference, Co-Organizer, Symposium: "Molecular Spectroscopy: Fundamental Research and Applications"
- 2015 - 2018 Editorial Board Member, Journal of Molecular Spectroscopy
- 2015 Pacificchem 2015, Co-organizer and Chairperson, Symposium: "Advances in Terahertz Spectroscopy & Imaging"
- 2014, 2018 DFG review panel: Priority Program "Dispersion"
- 2014 - 2015 Steacie Prize for Natural Sciences, Member of the Adjudication Panel
- 2013 - 2014 E.W.R. Steacie Memorial Fellowships Selection Committee
- 2013 Evaluation Committee, DFG Sonderforschungsbereich, Rostock, Germany
- 2012 - 2018 International Advisory Committee, International Conference on Quantum Fluid Clusters
- 2012 Laidler Award Selection Committee
- 2012 - 2020 International Advisory Committee, Chemistry and Physics at Low Temperatures
- 2011 - 2012 International Advisory Committee, International Matrix Symposium

## RESEARCH INTERESTS

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My research interests center around the study of weak intermolecular interactions. My group is using an integrated approach which involves both experimental and computational techniques to further our understanding of these van der Waals interactions. The experimental approach taken in my laboratory is to characterize van der Waals dimers, trimers, and higher clusters spectroscopically in the microwave and infrared frequency ranges. The rotational and ro-vibrational spectra that can be measured in these frequency ranges depend in a most sensitive way upon the particular interaction potential energy surface, and can be regarded as fingerprints of the intermolecular interactions. In addition, the study of isolated, size selected clusters, as opposed to bulk phase systems, has the advantage that three- and more-body non-additive interactions can be more easily extracted from the experimental results. In addition, we are generating high quality *ab initio* potential energy surfaces of weakly bound clusters to complement, and in some cases to facilitate, the experimental studies. Of current interest are hydration studies of volatile organic compounds that are precursors to organic atmospheric aerosol particles

Within the context of the 2002 NSERC Steacie Fellowship, my group has constructed a Helium Nanodroplet Isolation Spectrometer, the first of its kind in Canada. Our microwave experiments have provided new insights into the energy level structures of doped helium nanodroplets, which are interesting quantum solvated systems. The study of these mesoscopic systems will help to bridge the gap in our understanding between isolated molecular systems and the bulk phase.

Our smog chamber studies are focused in the studies of aerosol formation. In initial experiments, we have employed infrared laser and UV spectroscopy to monitor precursor gas

concentrations. During these experiments, we succeeded in the infrared spectroscopic, real-time detection of a reaction product. In our more recent experiments, we have studied the aging process of soot in the atmosphere and aerosol particle formation in the co-combustion of biomass and PVC.

SELECTED PUBLICATIONS (TOTAL NUMBER: 217)

- 1 AS Hazrah, CD Carlson, MH Al-Jabiri, Y Xu, and W Jäger, “Conformers of the  $\alpha$ -Pinene···Water Complex and Their Atmospheric Impacts: Insights from Rotational Spectroscopy.” *J. Phys. Chem. Lett.* **16**, 7359-7368 (2025).
- 2 J Ma, A Insausti, W Jäger, Y Xu, “Quantum Tunneling Fingerprints of Chirality-Induced Symmetry Preferences in Methyl Lactate Dimer.” *J. Am. Chem. Soc.* (2025).
- 3 S Beresnak, S Oswald, B Wu, NA Seifert, MA Suhm, W Jäger, and Y Xu, “Rotational and Vibrational Spectroscopy of a Weakly Bound Hexafluoroisopropanol···Dinitrogen Complex:  $^{14}\text{N}$  Hyperfine Splittings, Molecular Geometry, and Experimental Benchmarks.” *Phys. Chem. Chem. Phys.* **27**, 7905-7915 (2025).
- 4 J Lan, C Wang, M Li, C Duan, H Wang, J Chen, J-U Grabow, W Jäger, Y Xu, Q Gou: “Modulating the Amine- $\text{CO}_2$  Interaction Strength: Toward Efficient Carbon Capture.” *J. Phys. Chem. Lett.* **15**, 10661-10667 (2024).
- 5 X Tian, J Lei, T Gao, S Zou, X Wang, M Li, C Wang, J Chen, J-U Grabow, W Jäger, Q Gou: “Complex Dance of Molecules in the Sky: Choreography of Intermolecular Structure and Dynamics in the Cyclopentene- $\text{CO}_2$ - $\text{H}_2\text{O}$  Hetero Ternary Cluster.” *Angew. Chem. Int. Ed.* **63**, e202412406 - 1-7 (2024).
- 6 JC Whiteside, A Insausti, J Ma, AS Hazrah, W Jäger, Y Xu: “The Effect of Hyperconjugation and Hydrogen Bonding on the Conformers of Methylated Monosaccharides.” *Chem. Eur. J.* **30**, e202403166 (2024).
- 7 AS Hazrah, A Insausti, J Ma, M Al-Jabiri, W Jäger, Y Xu: “Wetting vs Droplet Aggregation: A Broadband Rotational Spectroscopic Study of 3-Methylcatechol···Water Clusters.” *Angew. Chem. Int. Ed.* **62**, e202310610 - 1-7 (2023).
- 8 J Qiang, L Zhou, P Lu, K Lin, Y Ma, S Pan, C Lu, W Jiang, F Sun, W Zhang, H Li, X Gong, ISh Averbukh, Y Prior, CA Schouder, H Stapelfeldt, IN Cherepanov, M Lemeshko, W Jäger, and J Wu: “Femtosecond rotational dynamics of  $\text{D}_2$  molecules in superfluid helium nanodroplets.” *Phys. Rev. Lett.* **128**, 243201 – 1-7 (2022).
- 9 AS Hazrah, S Nanayakkara, NA Seifert, E Kraka and W Jäger: “Structural Study of 1- and 2-Naphthol: New Insights into the Noncovalent H-H Interaction in *cis*-1-Naphthol.” *Phys. Chem. Chem. Phys.* **24**, 3722-3732 (2022).
- 10 AJ Feinberg, D Verma, SMO O’Connell-Lopez, S Erukala, RMP Tanyag, W Pang, CA Saladrigas, BW Toulson, M Borgwardt, N Shivaram, M-F Lin, A Al Haddad, W Jäger, C Bostedt, P Walter, O Gessner, and AF Vilesov: “Aggregation of solutes in bosonic versus fermionic quantum fluids.” *Sci. Adv.* **7**, eabk2247 - 1-5 (2021).
- 11 F Xie, M Fusè, AS Hazrah, W Jäger, V Barone, and Y Xu: “Discovering the Elusive Global Minimum in a Ternary Chiral Cluster: Rotational Spectra of Propylene Oxide Trimer.” *Angew. Chem. Int. Ed.* **59**, 22427-22430 (2020).
- 12 F Xie, NA Seifert, W Jäger and Y Xu: “Conformational Panorama and Chirality Controlled Structure–Energy Relationship in a Chiral Carboxylic Acid Dimer.” *Angew. Chem. Int. Ed.* **59**, 15703-15710 (2020).
- 13 NA Seifert, AS Hazrah, and W Jäger, “The 1-naphthol Dimer and its Surprising Preference for  $\pi$ - $\pi$  Stacking over Hydrogen Bonding.” *J. Phys. Chem. Lett.* **10**, 2836-2841 (2019).

- 14 S Oswald, NA Seifert, F Bohle, M Gawrilow, S Grimme, W Jäger, Y Xu, and MA Suhm, "The chirality-synchronized trimer of achiral hexafluoroisopropanol: A multi-messenger study." *Angew. Chem.* **58**, 5080-5084 (2019).
- 15 K Broda, JS Olfert, I Martin, G Schill, G McMeeking, EG Schnitzler, and W Jäger, "A Novel Inversion Method to Determine the Mass Distribution of Non-Refractory Coatings on Refractory Black Carbon using a Centrifugal Particle Mass Analyzer and Single Particle Soot Photometer." *Aerosol Sci. Technol.* **52**, 567-578 (2018). (2018 AST Editor's Choice)
- 16 KK Leung, EG Schnitzler, W Jäger, and JS Olfert, "Relative Humidity Dependence of Soot Aggregate Restructuring Induced by Secondary Organic Aerosol: Effects of Water on Coating Viscosity and Surface Tension." *Environ. Sci. Technol. Lett.* **4**, 386-390 (2017).
- 17 J Thomas, NA Seifert, W Jäger, and Y Xu, "A direct link from the gas to the condensed phase: A rotational spectroscopic study of 2,2,2-Trifluoroethanol trimers." *Angew. Chem.* **129**, 6386-6390 (2017) and *Angew. Chem. Int. Ed.* **56**, 6289-6293 (2017).
- 18 EG Schnitzler, C Badran, and W Jäger, "The Contrasting roles of water in the decarboxylation of two oxalic acid monohydrates: A combined rotational spectroscopic and ab initio study." *J. Phys. Chem. Lett.* **7**, 1143-1147 (2016).
- 19 J Thomas, X Liu, W Jäger, and Y Xu, "Unusual H-bond topology and bifurcated H-bonds in the 2-fluoroethanol trimer." *Angew. Chem.* **127**, 11877-11881 (2015) and *Angew. Chem. Int. Ed.* **54**, 11711-11715 (2015).
- 20 S Ghosh, J Thomas, W Huang, Y Xu, and W Jäger, "Rotational Spectra of Two Hydrogen-Bonded Methyl Salicylate Monohydrates: Relative Stability and Tunneling Motions." *J. Phys. Chem. Lett.* **6**, 3126-3131 (2015).
- 21 TMF Amin, MQ Huda, J Tulip, and W Jäger, "Design and Fabrication of a Long Arm Comb Drive Rotary Actuator with Externally Mounted Mirror for Optical Applications." *J. Microelectromech. S.* **24** 1565-1574 (2015).
- 22 EG Schnitzler, A Dutt, AM Charbonneau, JS Olfert, and W Jäger, "Soot aggregate restructuring due to coatings of secondary organic aerosol derived from aromatic precursors." *Environ. Sci. Technol.* **48**, 14309-14316 (2014).
- 23 J Thomas, W Jäger, and Y Xu, "Chirality induction and amplification in the 2,2,2-trifluoroethanol ••propylene oxide adduct." *Angew. Chem.* **126**, 7405-7408 (2014) and *Angew. Chem. Int. Ed.* **53**, 7277-7280 (2014).
- 24 J Thomas, O Sukhorukov, W Jäger, and Y Xu, "Direct Spectroscopic Detection of the Orientation of Free OH Groups in Methyl Lactate-(Water)(1,2) Clusters: Hydration of a Chiral Hydroxy Ester." *Angew. Chem.* **126**, 1175-1178 (2014) and *Angew. Chem. Int. Ed.* **53**, 1156-1159 (2014).
- 25 J Thomas, O Sukhorukov, W Jäger, and Y Xu, "Chirped pulse and cavity based FTMW spectra of the methyl lactate - ammonia adduct: lock and key selectivity and internal rotation motions." *Angew. Chem.* **125**, 4498-4501 (2013) and *Angew. Chem. Int. Ed.* **52**, 4402-4405 (2013).
- 26 PL Raston, W Jäger, H Li, RJ Le Roy, and PN Roy, "Observation of Persistent Molecular Superfluidity in para-Hydrogen Clusters." *Phys. Rev. Lett.* **108**, 253402 - 1-5 (2012).
- 27 L A Surin, A V Potapov, B S Dumesh, S Schlemmer, Y Xu, P L Raston, W Jäger, "Rotational Study of Carbon Monoxide Solvated with Helium Atoms." *Phys. Rev. Lett.* **101**, 233401 (2008).
- 28 ARW McKellar, Y Xu, W Jäger, "Spectroscopic Exploration of Atomic Scale Superfluidity in Doped Helium Nanoclusters." *Phys. Rev. Lett.* **97**, 183401 - 1-4 (2006).
- 29 Y Xu, W Jäger, J Tang, ARW. McKellar, "Spectroscopic Studies of Quantum Solvation in  ${}^4\text{He}_N\text{-N}_2\text{O}$  Clusters." *Phys. Rev. Lett.* **91**, 163401 - 1- 4 (2003).
- 30 J van Wijngaarden, W Jäger, "The  $\text{Ne}_3\text{-NH}_3$  van der Waals Tetramer: Rotational Spectra and ab initio Calculations." *J. Am. Chem. Soc.* **125**, 14631-14641 (2003).
- 31 J Tang, Y Xu, ARW. McKellar, W Jäger, "Quantum Solvation of Carbonylsulfide with Helium Atoms", *Science* **297**, 2030-2034 (2002).