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## EDUCATION

- 2005–2011 Ph.D. University of Georgia (Athens, GA, USA)  
*Ph.D. Dissertation title:* "Quantification of Virtual Chemical Properties: Strain, Hyperconjugation, Conjugation, and Aromaticity"  
*Advisor:* Professor Paul von Ragué Schleyer
- 2000–2004 B.S. Tung-Hai University (Taichung, Taiwan)

## PROFESSIONAL EXPERIENCE

- 2015–present Assistant Professor University of Houston (Houston, TX, USA)  
2013–2015 Research Scientist University of Georgia (Athens, GA, USA)  
2011–2013 Postdoctoral Associate University of Georgia (Athens, GA, USA)  
*Advisor:* Professor Paul von Ragué Schleyer

## HONORS AND AWARDS

- 2020 Sloan Research Fellowship  
2019 NIH-Maximizing Investigators' Research Award (MIRA) (R35)  
2018 NSF-CAREER Award  
2012 IUPAC-Solvay Prize for Young Chemist

## PUBLICATIONS *resulting from work performed at the University of Houston*

(Corresponding author(s) is indicated by \*)

78. Karas, L. J.; Campbell, A. T.; Alabugin, I. V.; **Wu, J. I.**\* "Antiaromaticity Gain Activates Tropone and Non-Benzenoid Aromatics as Normal-Electron-Demand Diels–Alder Dienes" *Org. Lett.* **2020** (accepted). DOI: 10.1021/acs.orglett.0c02343
77. Karas, L. J.; **Wu, J. I.**\* "Chapter 10: Antiaromaticity: A Brief History, Concepts, and Applications" in *Aromaticity: Modern Computational Methods and Applications* Elsevier. **2021** (accepted).
76. Karas, L. J.; Wu, C. H.;\* Ottosson, H.;\* **Wu, J. I.**\* "Electron-Driven Proton Transfer Relieves Excited-State Antiaromaticity in Photoexcited DNA Base Pairs" *Chem. Sci.* **2020** (accepted). DOI: 10.1039/D0SC02294B
75. Tran, T.; Karas, L. J.; Wu, J. I.; Do, L. H.\* "Elucidating Secondary Metal Cation Effects on Nickel Olefin Polymerization Catalysts" *ACS Catalysis* **2020** (accepted). DOI: 10.1021/acscatal.0c02949
74. Dressler, J. J.; Barker, J. E.; Karas, L. J.; Hashimoto, H. E.; Kishi, R.; Zakharov, L. N.; MacMillan, S. N.; Gomez-Garcia, C. J.; Nakano, M.; Wu, J. I.; Haley, M. M.\* "Late-Stage Modification of Electronic Properties of Antiaromatic and Diradicaloid Indeno[1,2-*b*]fluorene Analogues via Sulfur Oxidation" *J. Org. Chem.* **2020** (in press). DOI: 10.1021/acs.joc.0c01387
73. Wu, Y.; Wen, Z.; Wu, J. I.; Teets, T. S.\* "Efficient Deep Blue Platinum Acetylide Phosphors with Acyclic Diaminocarbene Ligands" *Chem. Eur. J.* **2020** (in press). DOI: 10.1002/chem.202002775

72. Paudel H. R.; Karas, L. J.; **Wu, J. I.**\* "On the Reciprocal Relationship Between  $\sigma$ -Hole Bonding and (Anti)aromaticity Gain in Ketocyclopolynes" *Org. Biomol. Chem.* **2020**, *18*, 5125-5129. DOI: 10.1039/D0OB01076F
71. Karas, L. J.; Wu, C. H.; Das, R.; **Wu, J. I.**\* "Hydrogen Bond Design Principles" *WIREs Comput. Mol. Sci.* **2020** (in press). DOI: 10.1002/wcms.1477
70. Wen, Z.; Karas, L. J.; Wu, C. H.; **Wu, J. I.**\* "How Does Excited-State Antiaromaticity Affect the Acidity Strengths of Photoacids?" *Chem. Commun. (Emerging Investigators Issue 2020)* **2020**, *56*, 8380-8383. DOI: 10.1039/D0CC02952A
69. Nhien, P. Q.; Chou, W. L.; Cuc, T. T. K.; Khang, T. M.; Wu, C. H.; Thirumalaivasan, N.; Hue, B. B.; **Wu, J. I.**; Wu, S. P.; Lin, H. C.\* " Multi-Stimuli Responsive FRET Processes of Bifluorophoric AIEgens in an Amphiphilic Copolymer and Its Application to Cyanide Detection in Aqueous Media" *ACS Appl. Mater. Interfaces* **2020**, *12*, 10959-10972. DOI: 10.1021/acsmi.9b21970
68. Paudel, H.; Das, R.; Wu, C. H.; **Wu, J. I.**\* "Self-Assembling Purine and Pteridine Quartets: How Do  $\pi$ -Conjugation Patterns Affect Resonance-Assisted Hydrogen Bonding" *Org. Biomol. Chem.* **2020**, *18*, 1078-1081. DOI: 10.1039/C9OB02412C
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66. Mu, G.; Wen, Z.; **Wu, J. I.**; Teets, T. S.\* "Azo-Triazolide Bis-Cyclometalated Ir(III) Complexes via Cyclization of 3-Cyanodiarylformazanate Ligands" *Dalton Trans.* **2020**, *49*, 3775-3785. DOI: 10.1039/C9DT03914G
65. Karas, L. J.; Wu, C. H.; **Wu, J. I.**\* "Computational Organic Chemistry" *Elsevier: Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, **2019**. DOI: 10.1016/B978-0-12-409547-2.10835-2
64. Uddin, M. N.; Knight, J. D.; Rastelli, E. J.; Soubra-Ghaoui, C.; Albright, T. A.; **Wu, J. I.**.\* Coltart, D. M.\* "On the Mechanism of the Asymmetric Aldol Addition of Chiral N-Amino Cyclic Carbamate Hydrazones: Evidence of Non-Curtin-Hammett Behavior" *Chem. Eur. J.* **2019**, *25*, 16037-16047. DOI: 10.1002/chem.201902388
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**PUBLICATIONS** resulting from work prior to UH appointment

(Corresponding author(s) is indicated by \*)

40. Jalife S.; **Wu, J. I.**; Martínez-Guajardo, G.; Schleyer, P. v. R.;\* Fernandez-Herra M. A.;\* Merino, G.\* "The Homocubyl Cation Rearrangement Revisited" *Chem. Commun.* **2015**, *51*, 5391-5393. DOI: 10.1039/c4cc08071h
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37. **Wu, J. I.**;\* Wang, C.; McKee W. C.; Schleyer, P. v. R.; Wei, W.; Mo, Y.\* "On the Large  $\sigma$ -Hyperconjugation in Alkanes and Alkenes" *J. Mol. Model.* **2014**, *20*, 2228. DOI: 10.1007/s00894-014-2228-2
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35. Zhu, C.; Luo, M.; Zhu, Q.; Schleyer, P. v. R.; **Wu, J. I.**; Lu, X.; Xia H.\* "Planar Möbius Aromatic Pentalenes Incorporating 16 and 18 Valence Electron Osmiums" *Nature Communications* **2014**, *5*, 3265. DOI: 10.1038/ncomms4265
34. Wu, C. H.; Galabov, B.;\* **Wu, J. I.**;\* Ilieva, S.; Schleyer, P. v. R.; Allen, W. D.\* "Do  $\pi$  Conjugative Effects Facilitate S<sub>N</sub>2 Reactions?" *J. Am. Chem. Soc.* **2014**, *136*, 3118-3126. DOI: 10.1021/ja4111946
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19. Shakib, F. A.;\* Momeni, M. R.; **Wu, J. I.**; Schleyer P. v. R.;\* Azizi, Z.; Ghambarian, M. "[n]Imperilene: Stacked [n]Trannulene Separated by Planar Cycloalkane Rings" *Org. Lett.* **2011**, *13*, 3600-3603. DOI: 10.1021/ol201216d
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7. **Wu, J. I.**; Wannere, C. S.; Mo, Y.; Schleyer, P. v. R.;\* Bunz, U. H. F.\* " $4n \pi$  Electrons but Stable: N,N-Dihydrodiazapentacenes" *J. Org. Chem.* **2009**, *74*, 4343-4349. DOI: 10.1021/jo900684c
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1. Miao, S.; Schleyer, P. v. R.; **Wu, J. I.**; Hardcastle, K. I.; Bunz, U. H. F.\* "A Thiadiazole-Fused N,N-Dihydroquinoxaline: Antiaromatic but Isolable" *Org. Lett.* **2007**, *9*, 1073-1076. DOI: 10.1021/ol070013i

#### INVITED CONFERENCE ORAL PRESENTATIONS

1. Wu, J. I. "TBA" Reaction Mechanisms Conference (RMC38), Denver, CO, USA; June 12–June 15, **2022**
2. Wu, J. I. "TBA" International Symposium on Novel Aromatic Compounds (ISNA), Warsaw, Poland; July 11–July 16, **2021**
3. Wu, J. I. "Molecules in a Hurry to Get Rid of Antiaromaticity" Pacificchem 2020: New Horizon of Main Group and Transition Metal Aromatics, Honolulu, HI, USA; Dec. 15–Dec. 20, **2020**
4. Wu, J. I. "Heteroatoms Here and There: Why it Matters for Designing  $\pi$ -Electronic Systems" Pacificchem 2020: Designed  $\pi$ -Electron Systems: Synthesis, Properties, Theory and Function, Honolulu, HI, USA; Dec. 15–Dec. 20, **2020**
5. Wu, J. I., 12<sup>th</sup> Triennial Congress of the World Association of Theoretical and Computational Chemists Vancouver, BC, Canada; August 16–21, **2020** (rescheduled to 2021)
6. Wu, J. I. "Excited-State Proton Transfer: Molecules in a Hurry to Get Rid of Antiaromaticity" International Conference on Horizons in Hydrogen Bond Research (HBOND19), Amsterdam, The Netherlands; Sept. 24–Sept. 27, **2019**

7. Wu, J. I. "*Excited-State Proton Transfer: Molecules in a Hurry to Get Rid of Antiaromaticity*" International Conference on Excited State Aromaticity and Antiaromaticity, Sigtuna, Sweden; July 29–Aug. 2, **2019**
8. Wu, J. I. "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*" Gordon Research Conference—Physical Organic Chemistry, Holderness, NH, USA; June 23–28, **2019**
9. Wu, J. I. "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*" Aromaticity 2018, Riviera Maya, Mexico; Nov. 28–Dec. 1, **2018**
10. Wu, J. I. "*Aromaticity-Modulated Noncovalent Interactions*" European Symposium on Chemical Bonding, Oviedo, Spain; Sept. 3–7, **2018**
11. Wu, J. I. "*Aromaticity-Modulated Hydrogen Bonding*" International Conference on Horizons in Hydrogen Bond Research (HBOND17), Jyväskylä, Finland; Sept. 10–14, **2017**
12. Wu, J. I. "*Aromaticity-Modulated Hydrogen Bonding*" World Association of Theoretical and Computational Chemists (WATOC) Satellite Meeting: The Chemical Bonds in the 21<sup>st</sup> Century Aachen, Germany; Sept. 2–4, **2017**
13. Wu, J. I. "*Aromaticity-Modulated Hydrogen Bonding*" Female Excellence in Theoretical Chemistry Putten, The Netherlands; June 22–25, **2017**
14. Wu, J. I. "*Achieving Short, Strong Hydrogen Bonds Through  $\pi$ -Conjugation Gain*" International Symposium of Chemical Sciences Houston, TX, USA; Jan. 19–21, **2017**
15. Wu, J. I. "*How do Enzymes Turn “Weak Acids” into Strong Proton Donors?*" Congress of the International Society of Theoretical and Chemical Physics 2016 Conference, Grand Forks, ND, USA; July 17–22, **2016**
16. Wu, J. I. "*How Can Weak Acids Be Strong Hydrogen Bond Donors?*" Solvay Meeting: Conceptual Quantum Chemistry, Brussels, Belgium; April 4–8, **2016**
17. Wu, J. I. "*Low-Barrier Hydrogen Bonding in Enzyme Catalysis*" Theory and Experiment: A Meeting at the Interface, Erlangen, Germany; March 30–April 1, **2016**
18. Wu, J. I. "*Tuning Hydrogen Bonds with Aromaticity*" Accelerating Organic Reaction Discovery Telluride, CO, USA; July 24–31, **2015**
19. Wu, J. I. "*Aromaticity Tomorrow: Concepts and Design in Silico*" International Conference on Chemical Bonding, Kauai, HI, USA; July 2–6, **2015**
20. Wu, J. I. "*Reconsidering Textbook Concepts of Carbocation Chemistry*" South Eastern Theoretical Chemistry Association Conference, University of Central Florida, FL, USA; May 14–6, **2015**

#### INVITED SEMINAR TALKS

1. Ohio State University, Department of Chemistry and Biochemistry, Columbus, OH, USA; Jan. 11, **2021** "TBA"
2. University of Campinas, Institute of Chemistry, Campinas, São Paulo, Brazil; August 20, **2020** "TBA"
3. Iowa State University, Department of Chemistry, Ames, IA, USA; March 6, **2019** "*Excited-State Proton Transfer: Molecules in a Hurry to Get Rid of Antiaromaticity*"
4. Swarthmore College, Department of Chemistry, Swarthmore, PA, USA; Feb. 6, **2019** "*Excited-State Proton Transfer: Molecules in a Hurry to Get Rid of Antiaromaticity*"
5. National Taiwan University, Center for Condensed Matter Sciences, Taipei, Taiwan; March 29, **2019** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"

6. National Chiao-Tung University, Department of Materials Science and Engineering, Hsinchu, Taiwan; March 27, **2019** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
7. Emory University, Department of Chemistry, Atlanta, GA, USA; March 6, **2019** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
8. University of Georgia, Department of Chemistry, Athens, GA, USA; March 5, **2019** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
9. University of Memphis, Department of Chemistry, Memphis, TN, USA; Nov. 16, **2018** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
10. University of California, Los Angeles, Department of Chemistry and Biochemistry, Los Angeles, CA, USA; Nov. 2, **2018** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
11. University of Oregon, Department of Chemistry and Biochemistry, Eugene, OR, USA; Oct. 31, **2018** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
12. University of California, Davis, Department of Chemistry, Davis, CA, USA; Oct. 30, **2018** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
13. University of North Texas, Department of Chemistry, Denton, TX, USA; Oct. 19, **2018** "*Aromaticity-Modulated Noncovalent Interactions: When Counting Electrons Matter*"
14. 2017-18 Assistant Professor Excellence Speaker Series (APeX), University of Houston, Houston, TX, USA; Jan. 31, **2018** "*Finding Magic Numbers in Chemistry—The Picasso Way*"
15. Leiden University, Chemical Biology Lecture Series, Leiden, The Netherlands; June 21, **2017** "*Aromaticity-Modulated Hydrogen Bonding*"

## CONTRIBUTED ORAL PRESENTATIONS

1. Wu, J. I. "*On the Nature of Low Barrier Hydrogen Bonds in Enzyme Catalysis*" International Conference on Horizons in Hydrogen Bond Research (HBOND15), Wrocław, Poland; September 13–18, **2015**.

## RESEARCH FUNDING

### Current Funding:

#### *Nation-wide Competition*

1. PI: Judy I. Wu  
 "*CAREER: Computational Studies of Aromaticity-Modulated Interactions in Supramolecular Chemistry*"  
 Sponsor: National Science Foundation  
 Amount: \$585,012  
 Funding period: 03/01/2018–02/28/2023
2. PI: Judy I. Wu  
 "*Computational Explorations of Unconventional Approaches to Control Noncovalent Interactions*"  
 Sponsor: National Institute of Health (Maximizing Investigators' Research Award, R35)  
 Amount: \$1,868,641  
 Funding period: 07/01/2019–06/30/2024
3. PI: Judy I. Wu  
 Sponsor: Alfred P. Sloan Research Fellowship  
 Amount: \$75,000



Funding period: 09/01/2020–08/31/2022

## RESEARCH MENTORING

### Postdoctoral Researchers

Chia-Hua Wu Fall 2015–present  
Ranjita Das Spring 2017–present

### Graduate Students

Mahsa Boraghi Spring 2017–Fall 2019 (Received M.S.)  
*M.S. thesis title:* "Computational Studies of Self-Assembling Squaramide and Urea Derivatives"  
Yu Zhang Fall 2016–Fall 2019 (Received M.S.)  
*M.S. thesis title:* "The Effects of Aromaticity Gain in Multipoint Hydrogen-Bonded Arrays"  
Hari Ram Paudel Spring 2016–Summer 2020 (Received Ph.D.)  
*Ph.D. dissertation title:* "Aromaticity-Modulated Interactions in Small Organic Molecules"

Zhili Wen Fall 2016–present  
Lucas Karas Fall 2017–present  
Siyeon Im Fall 2018–present

### Undergraduate Students

Krista van Rickley Fall 2015–Spring 2016  
Cindy Vasquez Fall 2015–Spring 2016  
Khanh Nguyen Fall 2016–Spring 2017

### High School Students

Michelle Lee Summer 2019  
Emily Gaw Summer 2017

### Student Accomplishments

Lucas Karas  
Jay K. Kochi Graduate Fellowship 2020  
NSM Graduate Student Profile 2020  
NSM Travel Award 2019  
Cullen Fellowship Travel Award 2019  
Graduate School Research Incentive Award 2018  
Zhili Wen  
Cullen Fellowship Travel Award 2019  
Yu Zhang  
Cullen Fellowship Travel Award 2017  
Chia-Hua Wu  
PCCP best poster prize at the *Second European Symposium of Chemical Bonding* 2018  
Postdoctoral Travel Award 2018

**COURSES TAUGHT**CHEM 4364: *Advanced Organic Chemistry*; Fall 2019, Fall 2017, Fall 2016CHEM 6312: *Bonding*; Spring 2020, Fall 2017, Fall 2016, Fall 2015**TEACHING EVALUATION SUMMARY***Scoring is out of 5, with a score of 5 being the highest.**Numbers in parentheses are the average values for comparable chemistry courses.*

Semester	Course	Students Enrolled	Students Responses	Mean Score for "Teaching Effectiveness"	Mean Overall Score
Spring 2020	CHEM 6312: <i>Bonding</i>	28	23	<b>4.48</b> (4.43)	<b>4.57</b> (4.50)
Fall 2019	CHEM 4364: <i>Advanced Organic Chemistry</i>	17	15	<b>4.53</b> (3.56)	<b>4.62</b> (3.72)
Fall 2017	CHEM 4364: <i>Advanced Organic Chemistry</i>	42	39	<b>4.36</b> (3.89)	<b>4.38</b> (4.10)
Fall 2017	CHEM 6312: <i>Bonding</i>	26	23	<b>4.39</b> (4.19)	<b>4.40</b> (4.22)
Fall 2016	CHEM 4364: <i>Advanced Organic Chemistry</i>	35	33	<b>4.60</b> (3.50)	<b>4.60</b> (4.20)
Fall 2016	CHEM 6312: <i>Bonding</i>	29	29	<b>4.80</b> (4.60)	<b>4.60</b> (4.60)
Fall 2015	CHEM 6312: <i>Bonding</i>	21	18	<b>4.72</b> (4.11)	<b>4.75</b> (3.89)

**SERVICE ACTIVITIES****Departmental Service***Member*, Graduate Admissions Committee (Fall 2017–present).*Member*, Bio-organic Chemistry Faculty Search Committee (2016).*Organic Division Seminar Coordinator* (Fall 2016–Spring 2017).*Departmental Seminar Coordinator* (Fall 2017–Spring 2018).*Member*: (Department of Chemistry, Department of Chemical and Biochemical Engineering)

- Oral Research Progress Committees,
- M.S. Thesis Committees,
- Ph.D. Dissertation Committees.

**In the Broader Scientific Community***Discussion Leader*, Gordon Research Conference–Physical Organic Chemistry (2017).*Manuscript Reviewer* (for 20+ journals), including:

*J. Am. Chem. Soc.*, *Chem. Commun.*, *J. Phys. Chem. Lett.*, *J. Org. Chem.*, *ACS Omega*, *J. Chem. Inf. Model*, *Can. J. Chem.*, *J. Phys. Chem. A*, *Org. Biomol. Chem.*, *Chem. Eur. J.*, *Tetrahedron*, *Scientific*

*Reports, J. Phys. Org. Chem., Org. Lett., Molecules, ChemPhysChem, New J. Chem., Int. J. Quant. Chem., RSC Advances, Chem. Phys. Lett., Phys. Chem. Chem. Phys., Acc. Chem. Res., Wiley Interdisciplinary Reviews, Nature Chemistry, Nature.*

*Grant Proposal Reviewer:*

American Chemical Society Petroleum Research Fund (ACS-PRF)  
National Science Foundation (NSF)  
National Institute of Health (NIH)  
Research Foundation Flanders (*Fonds Wetenschappelijk Onderzoek*)

*Mentor, Welch Summer Scholars Program (2017, 2019)*

*Selection Committee, Schleyer Lecture (2017–2019)*

*Advisory Board Member for Chemical Communications (2020–present)*

*Associate Editor for the Journal of Physical Organic Chemistry (2020–present)*