Juan J. Duchimaza Heredia

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Education

August 2018 — **PhD, Physical Chemistry**
Iowa State University, Ames, IA
Major professor: Dr. Mark S. Gordon
Dissertation title: *Going local: Exploring intricate bonding patterns with localized quasi-atomic orbitals*

May 2011 — **B.S., Chemistry and B.S., Computer Science**, *cum laude*
Honors Program minor
Ithaca College, Ithaca, NY

Professional Experience

2020-2021 — **Visiting Assistant Professor**, Emmanuel College, Boston, MA

2020 — **Science Teacher/Mentor**, Fusion Academy, Newton, MA

2018-2019 — **Postdoctoral Research Associate,** Boston University, Boston, MA

2012-2018 — **Graduate Research Assistant,** Iowa State University, Ames, IA

2012-2013 — **Graduate Teaching Assistant,** Iowa State University, Ames, IA

2012 — **Curriculum Developer,** iD Tech Camps, Campbell, CA

2011 — **Summer Instructor,** iD Tech Camps, Campbell, CA

Teaching Experience

Fall 2020 – Spring 2021 — **Emmanuel College Department of Physics and Chemistry**
CHEM 3105 and CHEM L3105: Physical Chemistry I: Thermodynamics w/ Lab,
CHEM 3106 and CHEM L3106: Physical Chemistry II: Quantum Mechanics w/ Lab,
CHEM L1101: Principles of Chemistry I Lab

Jan 2020 - present — **Fusion Academy Newton**
Science Teacher/Mentor
Teach science classes to middle and high school students in a one-to-one setting. Subjects covered include earth science, biology, chemistry, and physics.

Boston University Department of Chemistry

Fall 2018, Fall 2019 — CH111: Intensive General and Quantitative Analytical Chemistry 1. Guest Lecturer
Taught four lectures (two each semester) with original materials to a class of 60 students. Administered two exams.

Iowa State University Department of Chemistry

Spring 2013 – Fall 2015
General and Physical Chemistry Tutor
Privately tutored a total of seven undergraduate students in various levels of General Chemistry and four undergraduate students in Quantum Chemistry.

Spring 2013
Chem178: General Chemistry II. Head Teaching Assistant
Assisted in writing weekly quizzes and three exams and the respective keys. Conducted weekly supplementary staff meetings for Teaching Assistants. Guest lectured a class of 150 students.

Fall 2012
Chem167: General Chemistry for Engineering Students. Teaching Assistant
Lead two recitation sections of 24 students each. Proctored weekly quizzes and monthly exams.

Chem167L: Laboratory in General Chemistry for Engineering. Teaching Assistant
Supervised and instructed students in chemical laboratory techniques and data analysis. Emphasized the importance of communicating clearly and critically analyzing data.

iD Tech Camps

Mar. 2012 – Apr. 2012
iD Programming Labs 101. Curriculum Developer
Developed an introductory course in programming to teach high school students the basics of computer science, including data types, algorithms, and programming languages. Developed evaluation projects in Javascript, ActionScript, Java, C++, and Python.

Jun. 2011 – Jul. 2011
iPad and iPhone App Development. Summer Instructor
Lead two two-week sections of intensive iOS app development. Explained concepts of Computer Science, including control flow, sorting algorithms, and transformations, in Objective-C.

Research Experience

Sept. 2018 – Oct. 2019
Boston University, Boston, MA
Postdoctoral Research
Advisor: Dr. Qiang Cui
Combined the Natural Bond Orbital method with Density Functional based Tight Binding (DFTB) to evaluate the electronic structure predicted by DFTB compared to conventional Density Functional Theory, especially in bonding in transition metal complexes. Explored the role of interactions between residues from DRM2 with base pairs in DNA that lead to sequence dependent cytosine methylation using a combination of classical (force field) and QM/MM molecular dynamics. Applied long range corrected Time-Dependent DFTB to determine the nature of fluorescence in carbon nanodots, using replica exchange MD for accelerated conformational sampling.

May 2012 – Aug. 2018
Iowa State University, Ames, IA
Graduate Research
Advisor: Dr. Mark S. Gordon
Utilized an intrinsic orbital localization method to explore bonding of rare gas organic molecules and transition metal molecules, with a particular focus on representation of agostic-like M-H-Si interactions. Developed a systematic analysis of localized orbitals to automatically determine their chemical characteristics and roles in bonding within a molecule.

Aug. 2010 – May 2011 **Ithaca College,** Ithaca, NY
Undergraduate Research
Advisor: Dr. Vincent Deturi
Explored effective methods to study the keto-enol tautomeric equilibrium of acetylacetone in different solvent environments with varying polarity. Methods used include Fragment Molecular Orbital method and the Effective Fragment Potential method combined with continuum models.

Publications

"Multicolor Polymeric Carbon Dots: Synthesis, Separation and Polyamide Supported Molecular Fluorophore Emissions." Zhi, B.; Yao, X.; Wu, M.; Mensch, A.; Cui, Y.; **Duchimaza-Heredia, J. J.**, Deng, J.; Trerayapiwat, K.; Niehaus, T.; Nishimoto, Y.; Frank, B.; Zhang, Y.; Hamers, R. J.; Fairbrother, H.; Orr, G.; Murphy, C.; Cui, Q.; Haynes, C. *manuscript in preparation.*

"Analysis of Density Functional Tight Binding with Natural Bonding Orbitals." Lu, X.; **Duchimaza-Heredia, J.**; Cui, Q. *J. Phys. Chem. A*. 123, 34, 7439-7453 (2019).

"A Quasi-Atomic Analysis of Three-Center Two-Electron Zr–H–Si Interactions." **Duchimaza Heredia, J. J.**; Sadow, A. D.; Gordon, M.S. *J. Phys. Chem. A.* 122, 50, 9653-9669 (2018).

"Quasi-Atomic Bonding Analysis of Xe-Containing Compounds." **Duchimaza Heredia, J. J.**; Ruedenberg, K.; Gordon, M.S. *J. Phys. Chem. A.* 122, 3442 (2018)

"Identification and Characterization of Molecular Bonding Structures by ab initio Quasi-Atomic Orbital Analyses." West, A.; **Duchimaza Heredia, J. J.**; Gordon, M. S.; Ruedenberg, K. *J. Phys. Chem. A.* 121, 8884 (2017).

"Graduate College Climate Survey." Ogilvie, C. A.; Adams, C.; McKen, A. S.; Bittner, K.; Carney, D.; Douskey, D.; **Duchimaza Heredia, J. J.**; Hengesteg, P.; Hutchinson, C.; Campbell, C; and Harding, T. *Graduate College Reports*. 12 (2016).

"Lewis Base Mediated β-Elimination and Lewis Acid Mediated Insertion Reactions of Disilazido Zirconium Compounds." Yan, K.; **Duchimaza Heredia, J. J.**; Ellern A., Gordon, M. S.; Sadow, A. D. J. Am. Chem. Soc. 135, 15225 (2013).

Presentations

"A quasi-atomic perspective of three-center-two-electron Zr-H-Si interactions". **Juan Duchimaza Heredia**, KaKing Yan, Aaron Sadow, and Mark S. Gordon. Oral Presentation: 2015 Northeast Regional Meeting of the American Chemical Society, June 2015. Ithaca, NY.

"Intrinsic bonding patterns via localized orbitals." **Juan Duchimaza Heredia,** Aaron West, Michael Schmidt, Mark Gordon, and Klaus Ruedenberg. Oral Presentation: 249th ACS National Meeting & Exposition, March 2015. Denver, CO.

"Computational insights into intramolecular hydrogen migration via agostic-type interactions." **Juan Duchimaza Heredia**, KaKing Yan, Arkady Ellern, Aaron Sadow, and Mark Gordon. Poster Presentation: 249th ACS National Meeting & Exposition, March 2015. Denver, CO.

"Keto-enol tautomerism of acetyl acetone: Modeling solvent effects using the effective fragment potential." **Juan Duchimaza**, Jade Pratt, and Vincent DeTuri. Poster Presentation: 241st ACS National Meeting & Exposition, March 2011. Anaheim, CA.

"Keto-enol tautomerism of acetyl acetone: Modeling solvent effects using the effective fragment potential". **Juan Duchimaza**. Oral Presentation: 25th National Conference for Undergraduate Research, March 2011. Ithaca College, Ithaca, NY.

"IC Network View Project". Allison Boos, Blake Balick-Schreiber, **Juan Duchimaza**, Evan Hong, Marc Howard, Richard Roberts, Jared Vinci, and Drew Winston. Oral Presentation: 25th National Conference for Undergraduate Research, March 2011. Ithaca College, Ithaca, NY.

Awards and Honors

2016	Gilman Award for Excellence in Chemistry, Iowa State University Chemistry Department
2015	Outstanding Teaching Award, Iowa State University Chemistry Department
	Frank J Moore and Thoreen Beth Moore Scholarship, Iowa State University Chemistry Department
2014	PennApps Spring 2014 Hackathon Participant, University of Pennsylvania, Philadelphia PA
2013	Third Place Award at Startup Weekend Des Moines Hackathon, Des Moines, IA

Additional Education and Training

2019	An Introduction to Evidence-Based Undergraduate STEM Teaching edX Inc. (MOOC Platform) Fall
2016	Gr St 586: Preparing Future Faculty Intermediate Seminar Iowa State University, Ames, IA Spring
2015	Gr St 585: Preparing Future Faculty Introductory Seminar Iowa State University, Ames, IA Fall
2014	Supercomputing 2014 Conference 16 November – 20 November
	Software-Development Summer School for Computational Chemistry and Materials Modeling Sustainable Software Innovation Institute for Computational Chemistry and Materials Modeling [$(SICM)^2$] 7 July – 18 July
2011	Stanford Artificial Intelligence online class 10 October – 16 December
	Stanford Machine Learning online class 10 October – 16 December

Leadership

Aug. 2015 – Jul. 2017	Latina/o Graduate Student Association (LGSA) President
Aug. 2013 – Jul. 2015	Latina/o Graduate Student Association (LGSA) Treasurer
Aug. 2013 – May 2017	Graduate and Professional Student Senate (GPSS) Chemistry Senator *Graduate and Professional Research Conference Committee, Professional Advancement Grants Committee, Rules Committee*
Aug. 2012 – May 2015	Iowa State Computer Science and Engineering Club Member

Service

Jan. 2017 – July 2018	Latinx Student Leader Affinity Council Co-Founder, Member Co-Chairs: Dr. Eliseo De Leon and Dr. Consuelo Liz Mendez-Shannon
Nov. 2015 – Feb. 2016	Iowa State University Strategic Planning, Student Experience Subcommittee Member Co-Chairs: Steve Mickelson and Rachel Wagner
Aug. 2014 – May 2015	Chemistry Graduate Student Liaison Committee Member Faculty advisor: Dr. Emily A. Smith

Affiliations

National Residence Hall Honorary
Upsilon Pi Epsilon (Computer Science Honor Society)
Society for Advancement of Chicanos/Hispanics and Native Americans in Science

Programs, Software, and Related Computer Skills

Chemistry: GAMESS, Gaussian, CHARMM, DFTB+, ChemDraw, VMD, MacMolPlt
Programming: Java, C++, Python, Fortran, Bash, LaTeX, HTML