

John C. Thomas

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Education

2008–2015 **University of California, Los Angeles**

Physical Chemistry Ph.D

Paul S. Weiss Group

Department of Chemistry & Biochemistry

California NanoSystems Institute

2005–2008 **University of Texas at San Antonio**

Chemistry B.S.

Department of Chemistry

Experience

Oct 2023– **Research Associate**, DARTMOUTH COLLEGE

Ongoing Thayer College of Engineering.

- Supervised between Prof. Geoffroy Hautier and Dr. Alexander Weber-Bargioni.
- Lead low-temperature scanning probe researcher on LT-AFM/STM with THz optical access, superconducting magnetic coil, and a microwave antenna.
- Installation, operation, and maintenance of two Createc UHV microscopes.
- Design and implementation of free-space optics.
- Maintain github libraries required for SPM experimental workflows, data analysis software development kits, and applied machine learning.

Oct 2023– **Research Affiliate**, LAWRENCE BERKELEY NATIONAL LABORATORY

Ongoing Molecular Foundry & Materials Science Division.

- Enable collaborative opportunities for Molecular Foundry users across the globe.
- Scanning probe activity manager and safety lead.
- Train users for experiments on the SPM with a quantum science focus.

Mar **Postdoctoral Fellow**, LAWRENCE BERKELEY NATIONAL LABORATORY

2020–Sep Molecular Foundry & Materials Science Division.

2023 ○ Alexander Weber-Bargioni Group.

- Lead low-temperature scanning probe researcher.
- Funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences.
- Operation and maintenance of a Createc UHV microscope.
- Execute user projects from collaborators across local and international institutions.
- Train postdoctoral scholars and students.
- Implement tool automation and lead web development.

Dec **Software Developer**, VERITOMYX, INC

2018–Feb SDK developer.

- 2020
- Implement API integration functionality within software development kits (SDKs) for mass spectrometer analytics and customer platform.
 - Contribute towards software solutions and systems design.

Sep **Process Technology & Development Engineer**, INTEL CORPORATION

2015–Nov Defect metrology & yield analysis.

- 2018
- Inline and end of line monitoring of silicon processes for server and IOT products, aimed at maximizing yield and reducing defectivity at multiple steps.
 - HVM data analysis geared towards identifying and creating solutions for particle minimization and product design issues.
 - Used process flow knowledge with problem solving skills in three-dimensional device design for HPC and SRAM.
 - Enabled timely communication on tool matching with website reporting schemes and daily directed taskforce meetings.
 - Trained and used statistical methods & design of experiments in tasks requested.

- Sep 2010–Sept 2015 **Graduate Researcher.** CALIFORNIA NANOSYSTEMS INSTITUTE
- Scanning Probe Microscopy.
- Conducted research on numerous projects detailing the functional control and placement of single-molecules.
 - Created new imaging and analysis procedures.
 - Operated custom-built and vendor-provided scanning probe microscopes held at liquid helium temperatures and in ambient conditions.
 - Designed, machined, and installed custom parts that were fabricated in the physics machine shop.
 - Collaborated across multiple disciplines.
 - Trained post doctoral scholars, graduate students, and undergraduate students on LTSPM.

Research Interests

Quantum Information Science: Working at the intersection of chemistry, physics, and materials science provides a unique perspective that can be used to identify and screen defects, materials, and molecules for use in quantum communication, computation, and sensing.

Artificial Intelligence and Machine Learning: The task of automating complex discovery and operational workflows can be achieved through the application of supervised, unsupervised, and active learning methods, where both labeled and unlabeled datasets can help fine tune models with utilization in autonomous discovery.

Surface Science: Scanning probe microscopy has made vast impact within the nanoscience field and has been extended to understand quasiparticle phenomena at the relevant length and time scales necessary to capture the insight necessary to design and build devices from the bottom-up, image the electronic and structural landscape of relevant semiconductor and optoelectronic materials, and to even visualize peptide formation at the picometer scale.

Journal Articles

1. **J. C. Thomas**, W. Chen, Y. Xiong, B. Barker, J. Zhou, W. Chen, A. Rossi, N. Kelly, Z. Yu, D. Zhou, S. Kumari, E. Barnard, J. Robinson, M. Terrones, A. Schwartzberg, D. F. Ogletree, E. Rotenberg, M. M. Noack, S. Griffin, A. Raja, D. Strubbe, G.-M. Rignanese, A. Weber-Bargioni, G. Hautier. "A substitutional quantum defect in WS₂ discovered by high-throughput computational screening and fabricated by site-selective STM manipulation." *Nature Communications* **15**, 3556 (2024).
2. A. Rossi, R. Dettori, C. Johnson, J. Balgley, **J. C. Thomas**, L. Francaviglia, R. Dettori, A. Schmid, K. Watanabe, T. Taniguchi, M. Cothrine, D. G. Mandrus, C. Jozwiak, A. Bostwick, E. Henriksen, A. Weber-Bargioni, and E. Rotenberg. "Direct Visualization of the Charge Transfer in a Graphene/ α -RuCl₃ Heterostructure via Angle-Resolved Photoemission Spectroscopy." *Nano Letters* **23**, 8000 (2023).
3. J. Zhou, **J. C. Thomas**, E. Barré, E. Barnard, A. Raja, S. Cabrini, K. Munechika, A. Schwartzberg, A. Weber-Bargioni. "Near-Field Coupling with a Nanoimprinted Probe for Dark Exciton Nanoimaging in Monolayer WSe₂." *Nano Letters* **23**, 4901 (2023).
4. **J. C. Thomas** & A. Rossi, J. T. Küchle, E. Barré, Z. Yu, D. Zhou, S. Kumari, H.-Z. Tsai, E. Wong, C. Jozwiak, A. Bostwick, J. A. Robinson, M. Terrones, A. Raja, A. Schwartzberg, D. F. Ogletree, J. B. Neaton, M. F. Crommie, F. Allegretti, W. Auwärter, E. Rotenberg, A. Weber-Bargioni. "WS₂ Band Gap Renormalization Induced by Tomonaga Luttinger Liquid Formation in Mirror Twin Boundaries." arXiv:2301.02721, (2023).
5. **J. C. Thomas**, A. Rossi, D. Smalley, L. Francaviglia, Z. Yu, T. Zhang, S. Kumari, J. A. Robinson, M. Terrones, M. Ishigami, E. Rotenberg, E. S. Barnard, A. Raja, E. Wong, D. F. Ogletree, M. M. Noack, A. Weber-Bargioni. "Autonomous Scanning Probe Microscopy Investigations over WS₂ and Au{111}." *npj Computational Materials* **8**, 99 (2022).
6. D. P. Goronzy, J. Staněk, E. Avery, H. Guo, Z. Bastl, M. Dušek, N. M. Gallup, S. Gün, M. Kučeráková, B. J. Lewandowski, J. Macháček, V. Šicha, **J. C. Thomas**, A. Yavuz, K. N. Houk, F. M. Daniman, E. Mete, A. N. Alexandrova, T. Baše, and P. S. Weiss. "Influence of Terminal Carboxyl Group on the Structure and Reactivity of Functionalized *m*-Carboranethiolate Self-Assembled Monolayers." *Chemistry of Materials* **32**, 6800 (2020).
7. **J. C. Thomas**, D. P. Goronzy, A. C. Serino, H. Auluck, O. Irving, W. Jimenez-Izal, J. Deirmenjian, J. Macháček, P. Sautet, A. Alexandrova, T. Baše, and P. S. Weiss. "Acid-Base Control of Valency within Carboranethiol Self-Assembled Monolayers: Molecules Do the Can-Can." *ACS Nano* **12**, 2211 (2018).
8. **J. C. Thomas**, D. P. Goronzy, K. Dragomiretskiy, D. Zosso, J. Gilles, S. J. Osher, A. L. Bertozzi, and P. S. Weiss. "Mapping Buried Hydrogen-Bonding Networks." *ACS Nano* **10**, 5446 (2016).
9. M. L. Gethers, **J. C. Thomas**, S. Jiang, N. O. Weiss, X. Duan, W. A. Goddard, III, and P. S. Weiss. "Holey Graphene as a Weed Barrier for Molecules." *ACS Nano* **9**, 10909 (2015).
10. **J. C. Thomas**, I. Boldog, H. S. Auluck, P. J. Bereciartua, M. Dušek, J. Macháček, Z. Bastl, P. S. Weiss, and T. Baše. "Self-Assembled *p*-Carborane Analog of *p*-Mercaptobenzoic Acid on Au{111}." *Chemistry of Materials* **27**, 5425 (2015).
11. **J. C. Thomas**, J. J. Schwartz, J. N. Hohman, S. A. Claridge, H. S. Auluck, A. C. Serino, A. M. Spokoiny, G. Tran, K. F. Kelly, C. A. Mirkin, J. Gilles, S. J. Osher, and P. S. Weiss. "Defect-Tolerant Aligned Dipoles within Two-Dimensional Plastic Lattices." *ACS Nano* **9**, 4734 (2015).
12. J. N. Hohman, **J. C. Thomas**, Y. Zhao, H. Auluck, M. Kim, W. Visselaar, S. Kommeren, A. Terfort, and P. S. Weiss. "Exchange Reactions between Alkanethiolates and Alkaneselenols on Au{111}." *Journal of the American Chemical Society* **126**, 8110 (2014).
13. J. Kim, Y. S. Rim, Y. Liu, A. C. Serino, **J. C. Thomas**, H. Chen, Y. Yang, and P. S. Weiss. "Interface Control in Organic Electronics Using Mixed Monolayers of Carboranethiol on Isomers." *Nano Letters* **14**, 2946 (2014).
14. S. A. Claridge, **J. C. Thomas**, M. A. Silverman, J. J. Schwartz, Y. Yang, C. Wang, and P. S. Weiss. "Differentiating Amino Acid Residues and Side Chain Orientations in Peptides Using Scanning Tunneling Microscopy." *Journal of the American Chemical Society* **135**, 18528 (2013).
15. S. A. Claridge, W.-S. Liao, **J. C. Thomas**, Y. Zhao, H. H. Cao, S. Cheunkar, A. C. Serino, A. M. Andrews, and P. S. Weiss. "From the Bottom Up: Dimensional Control and Characterization in Molecular Monolayers." *Chemical Society Reviews* **42**, 2725 (2013).
16. Y. B. Zheng, B. K. Pathem, J. N. Hohman, **J. C. Thomas**, M. H. Kim, and P. S. Weiss. "Photoresponsive Molecules in Well-Defined Nanoscale Environments." *Advanced Materials* **25**, 302 (2013).
17. J. N. Hohman, M. Kim, B. Schüpbach, M. Kind, **J. C. Thomas**, A. Terfort, and P. S. Weiss. "The Dynamic Double Lattice of 1-Adamantaneselenolate Self-Assembled Monolayers on Au{111}." *Journal of the American Chemical Society* **133**, 19422 (2011).
18. **J. C. Thomas**, E. R. Tieckink, J. A. Walmsley. "[4'-(4-Aminophenyl)-2,2':6',2''-terpyridine] chloridopalladium (II) chloride." *Acta Crystallographica Section E: Structure Reports Online* **67**, m733 (2011).
19. A. R. Kurland, P. Han, **J. C. Thomas**, A. N. Giordano, and P. S. Weiss. "Adsorbate-Promoted Tunneling-Electron- Induced Local Faceting of D/Pd110-(1×2)." *Journal of Physical Chemistry Letters* **1**, 2288 (2010).

Submitted or In Preparation

1. K. E. White, Y. Chu, G. Gani, S. Ippolito, K. Barr, **J. C. Thomas**, A. Weber-Bargioni, K. Lau, Y. Gogotsi, P. S. Weiss. "Atomic-scale investigations of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene surfaces." *in review*.

Book Chapter

1. A. Rossi, D. Smalley, M. Ishigami, E. Rotenberg, A. Weber-Bargioni, and **J. C. Thomas**. "Autonomous Hyperspectral Scanning Tunneling Spectroscopy," *Taylor & Francis* 2023, Chapter 12 ISBN 978-1032314655 (DOI: 10.1201/9781003359593).

Thesis

J. C. Thomas. "Probing Buried and Exposed Interfaces with Submolecular Precision." Advisor - Paul S. Weiss (2015). [link](#)

Presentations

Invited

1. "Controlling Quasiparticle Excitations in 2D Solids Through Atomically Precise Heterostructures." **J. C. Thomas**. MRS Fall Meeting, Boston, MA (2023).
2. "Quantum Defects by Design in 2D Materials: Routes for Pairing Experiment with High-Throughput Screening and Autonomous Discovery." **J. C. Thomas**. Rice University Nanoscale Imaging Series (2023).
3. "Machine-Driven Applications in Scanning Probe Microscopy at the Atomic Scale." **J. C. Thomas**. Autonomous Discovery in Science and Engineering, Lawrence Berkeley National Laboratory (2021).
4. "Machine Learning in Scanning Probe Microscopy." **J. C. Thomas**. Berkeley Lab's Energy Sciences Area, Science Hour, Lawrence Berkeley National Laboratory (2021).

Contributed

1. "Quantum Defect Candidates at Modified Substitution Sites within WS_2 ." **J. C. Thomas**. MRS Fall Meeting, Boston, MA (2023).
2. "Band gap renormalization across 1D mirror twin boundaries in WS_2 ." **J. C. Thomas**. ACS Fall Meeting, San Francisco, CA (2023).
3. "Defect Implementation in 2D vdW Materials: Highly Correlated Fermion States and Autonomous Experimentation." **J. C. Thomas**, A. Weber-Bargioni. Graphene, Manchester, UK (2023).
4. "One-Dimensional Bose Gas within Mirror Twin Boundary Formations in WS_2 ." **J. C. Thomas**. MRS Spring Meeting, San Francisco, CA (2023).
5. "Artificially Intelligent Investigations on Transition Metal Dichalcogenides with Scanning Probe Microscopy." **J. C. Thomas**. ACS Spring Meeting, Indianapolis, IN (2023).
6. "Tomonaga-Luttinger Liquid Formation in Mirror Twin Boundaries within WS_2 ." **J. C. Thomas**. APS March Meeting, Las Vegas, NV (2023).
7. "Hyperspectral Scanning Tunneling Spectroscopy over WS_2 and $\text{Au}\{111\}$ " **J. C. Thomas**. ECOS35, Luxembourg, Luxembourg (2022).
8. "Transition Metal Dichalcogenide Defect Functionalization with Magnetic Impurities – Defect Introduction and Identification." **J. C. Thomas**. MRS Spring Meeting, Honolulu, HI (2022).
9. "Scanning Probe Characterization over Defective WS_2 and $\text{Au}\{111\}$." **J. C. Thomas**, A. Rossi, D. Smalley, L. Francaviglia, Z. Yu, T. Zhang, S. Kumari, J. Robinson, M. Terrones, M. Ishigami, E. Rotenberg, E. Barnard, A. Raja, E. Wong, D. F. Ogletree, M. M. Noack, A. Weber-Bargioni. APS March Meeting, Chicago, IL (2022).
10. "Machine-Driven Characterization and Classification over Au and WS_2 ." **J. C. Thomas**. Machine Learning and Automated Experiment in Scanning Probe Microscopy, Virtual School, Oak Ridge National Laboratory (2021).
11. "Defect Engineering within Transition Metal Dichalcogenides Using Magnetic and Rare-Earth Metals." **J. C. Thomas**, K. A. Cochrane, A. Weber-Bargioni. APS March Meeting (2021).
12. "Mapping Locally Aligned Dipoles within Two-Dimensional Plastic Lattices and Majority Thiol vs Thiolate Control in Carboranedithiolate Monolayers." **J. C. Thomas**, J. J. Schwartz, H. Auluck, B. M. Matthews, J. Dermenjian, G. Tran, A. Bertozzi, J. Gilles, S. Osher, C. A. Mirkin, T. Baše, P. S. Weiss. International Conference on Nanoscience and Technology (ICN+T), Vail, CO, USA (2014).
13. "Mapping Local Dipole Moments within Two-Dimensional Plastic Lattices." **J. C. Thomas**, J. J. Schwartz, H. S. Auluck, G. Tran, J. Gilles, S. Osher, C. A. Mirkin, P. S. Weiss. 60th American Vacuum Society International Symposium. Probe-Sample Interactions, Nano-Manipulation and Emerging Instrument Formats Session, Long Beach, CA, USA (2013).

Poster

1. "Engineered Defects within Tungsten Disulfide: Candidates for Atomic Scale Quantum Emitters." **J. C. Thomas**, A. Weber-Bargioni. Quantum Systems Accelerator All Hands Meeting, Berkeley, CA, USA (2023).
2. "Autonomous Hyper Scanning Tunneling Spectroscopy." **J. C. Thomas**, M. M. Noack, A. Weber-Bargioni. UCLA IPAM: Multi-Modal Imaging with Deep Learning and Modeling, Los Angeles, CA, USA (2022).
3. "Engineering Local Quantum States via the Introduction of 0D and 1D Defects in 2D Materials." **J. C. Thomas**, A. Weber-Bargioni. molQueST, Ascona, Switzerland (2022).
4. "Defect Engineering within Transition Metal Dichalcogenides and Machine Learning Approachs towards STM/STS Tip Shaping on Au." **J. C. Thomas**, K. A. Cochrane, A. Weber-Bargioni. Graphene, Virtual (2020).
5. "Beneath and Between: Structural, Functional, and Spectroscopic Measurements of Buried Interfaces and Interactions." **J. C. Thomas**, P. S. Weiss. Electron and Scanning Probe Microscopies Principal Investigator's Meeting, Gaithersburg, MD, USA (2014).
6. "Visualizing Assembly of Differently Oriented Dipole Moments within Carboranethiols on Metal Substrates." B. Matthews, **J. C. Thomas**, H. S. Auluck, L. A. Stewart, P. S. Weiss. Annual Biomedical Research Conference for Minority Students [ABRCMS], Nashville, TN, USA (2013).
7. "Difunctionalized Carboranes on Gold Surfaces" O. Irving, **J. C. Thomas**, H. S. Auluck, J. Dadras, A. Alexandrova, P. S. Weiss. Glenn T. Seaborg Symposium, UCLA (2013).
8. "Probing the Buried and Exposed Interface within Two-Dimensional Structures." **J. C. Thomas**, P. S. Weiss. Glenn T. Seaborg Symposium, UCLA (2013).
9. "Analyzing Complex Self-Assembled Systems: A Combined Approach based on Microwave-modulated Scanning Tunneling Microscopy and Large-Scale Molecular Modeling." S. A. Claridge, **J. C. Thomas**, J. J. Schwartz, M. S. Silverman, Y. Yang, C. Wang, P. S. Weiss. 244th ACS National Meeting & Exposition, Philadelphia, PA, USA (2012).
10. "Imaging and Single-Molecule Vibrational Spectroscopy of Cubanethiolate on Au{111}." **J. C. Thomas**, J. N. Hohman, H. S. Auluck, M. Kim, J. R. Griffiths, R. Priefer, P. S. Weiss. 243rd ACS National Meeting & Exposition, San Diego, CA, USA (2012).
11. "Heavy Metal Complexes of 4'-(4-Aminophenyl)-2,2':6',2"-terpyridine." **J. C. Thomas**, E. R. T. Tienkink, J. A. Walmsley. 235th ACS National Meeting& Exposition, New Orleans, LA, USA (2008).

Teaching

Sept **Adjunct Instructor**

2019–Mar *Clark College*

2020 *Department of Chemistry*

- Taught lecture and lab sections for concepts in chemistry and an allied health chemistry course (Chem 110 & Chem 112) that both highlighted general chemistry subjects.
- Courses consisted of about 36 students per discussion and separated into two lab sections (18 students each).
- Duties included creating exams, homework, group activities, quizzes, and organizing online materials.
- Automated class reports and individualized course statistics.

Jan **Adjunct Instructor**

2020–Mar *Clackamas Community College*

2020 *Department of Chemistry*

- Taught lab sections for both general chemistry and introduction to chemistry.
- Authored class reports and individualized course statistics.

Oct **Teaching Assistant**

2011–Aug *Discussion & Lab Lead*

2012 *University of California, Los Angeles*

Department of Chemistry & Biochemistry

- Introduction to Quantum Mechanics (Chem 113A).
- Chemical Thermodynamics (Chem 110A).
- General and Organic Chemistry Laboratory Series (Chem 14L).

Aug **Undergrad Teaching Assistant**

2007–Dec *University of Texas at San Antonio*

2007 *Department of Chemistry*

- Organic Chemistry Laboratory Series (CHE 2612 & CHE 3652).

Mentoring & Outreach

- 2022-2023 **APS Career Mentoring Fellow**
American Physical Society
Mentored and interacted with numerous APS members regarding careers in physics and engineering after graduate school or a postdoctoral appointment.
- 2022-
Ongoing **Berkeley Lab Mentor**
MESA Program
Mentored incoming technicians at Lawrence Berkeley National Lab focused on career planning within the scope of assisting for success in science and innovation.
- 2012-2015 **High School Student Mentor**
Marlborough School
Served as a mentor for two high school students working on self-assembled materials projects ranging from instrumentation to data analysis.
- 2012-2015 **Undergraduate Student Mentor**
UCLA CARE-SEM Program
Mentored two undergraduate students on self-assembled materials and molecular modeling projects. Helped them to create research summaries, posters, and ultimately present at national conferences.
- 2013-2015 **Lead/Participant**
CNSI High School Nanoscience Program
The program teaches high school teachers how to perform nanoscience experiments and how to teach the experiment in their classrooms. Lead the superhydrophobics experiment and participated in several others. Duties as lead are to train new graduate student volunteers on the experiment, organize the experiment for the teachers, and present the experimental background and results.
- 2014 **Judge**
Los Angeles County Science Fair
Acted as a judge for high school juniors in a science fair by questioning the students about their projects. As part of a team, the top three chemistry related science projects were chosen.
- 2010 **Undergraduate Student Mentor**
CSST Program
Mentored international undergraduate students on two-dimensional nanoparticle formation projects at UCLA.

Affiliations

American Chemical Society
American Vacuum Society
Materials Research Society
American Physical Society
Molecular Foundry
Advanced Light Source
California NanoSystems Institute
University of Münster, Department of Physics - Visiting researcher
NPJ Computational Materials - Journal Referee
Communications Physics - Journal Referee
Ultramicroscopy - Journal Referee
Patterns - Journal Referee
Frontiers in Materials | Quantum Materials - Review Editor
Royal Society of Chemistry (PCCP) – Journal Referee
Beilstein Journal of Nanotechnology – Journal Referee

Software

- 2022-present **Principal Developer of gpSTS**
Molecular Foundry, Lawrence Berkeley National Laboratory.

Skills

Techniques	Scanning tunneling microscopy, atomic force microscopy, optical spectroscopy, photoelectron spectroscopy, infrared spectroscopy, transmission and scanning electron microscopies, physical evaporation, low-energy electron diffraction, nuclear magnetic resonance spectroscopy, machine shop training, instrumentation problem-solving, clean room training
Languages	Python, C/C++, Java, SQL, JMP, LabVIEW, Matlab, Perl
Frameworks	PyTorch, gpCAM, pymatgen
WebDev	HTML/CSS, JavaScript, PHP
Utility	Git, Jupyter Notebook
Graphics	POV-Ray, Adobe, Blender
Application	VASP, AutoCAD, SolidWorks
Communication	English

Awards

2023	SPOT Award Lawrence Berkeley National Laboratory
2021-2022	Energy Frontier Research Center Post Doctoral Fellowship Lawrence Berkeley National Laboratory
2013-2014	W. M. Keck Foundation Fellow University of California, Los Angeles
2008-2010	Bunton-Waller Fellowship The Pennsylvania State University
2007-2008	MBRS-RISE Fellowship University of Texas at San Antonio

References

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