

# 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, Biology* B.S.

Departments of Chemistry & Biology

## Experience

Mar 2020– **EFRC Postdoctoral Fellow**, LAWRENCE BERKELEY NATIONAL LABORATORY

Ongoing Molecular Foundry & Materials Science Division.

- 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.

## 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.

## Publications (Google Scholar)

### Journal Articles

1. **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 WS<sub>2</sub> and Au{111}." *NPJ Computational Materials* **8**, 99 (2022).
2. 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).
3. **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 Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can." *ACS Nano* **12**, 2211 (2018).
4. **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).
5. 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).
6. **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).
7. **J. C. Thomas**, J. J. Schwartz, J. N. Hohman, S. A. Claridge, H. S. Auluck, A. C. Serino, A. M. Spokoyny, 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).
8. J. N. Hohman, **J. C. Thomas**, Y. Zhao, H. Auluck, M. Kim, W. Vijselaar, 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).
9. 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).
10. 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).
11. 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).
12. 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).
13. 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).
14. **J. C. Thomas**, E. R. Tiekink, J. A. Walmsley. "[4'-(4-Aminophenyl)-2,2':6',2''-terpyridine] chloridopalladium (II) chloride." *Acta Crystallographica Section E: Structure Reports Online* **67**, m733 (2011).
15. 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. J. Zhou, E. Barré, **J. C. Thomas**, A. Raja, K. Munechika, E. Barnard, A. Schwartzberg, A. Weber-Bargioni, S. Cabrini. "Near-field optical mapping of dark excitons in WSe<sub>2</sub> monolayer." *in preparation*.
2. **J. C. Thomas** & A. Rossi, J. T. Küchle, E. Barré, Z. Yu, T. Zhang, S. Kumari, H.-Z. Tsai, J. A. Robinson, M. Terrones, E. S. Barnard, A. Raja, E. Wong, D. F. Ogletree, F. Allegretti, M. F. Crommie, W. Auwärter, E. Rotenberg, A. Weber-Bargioni. "Defective States within WS<sub>2</sub>." *in preparation*.

### Book Chapter

1. **J. C. Thomas**, A. Rossi, D. Smalley, M. Ishigami, E. Rotenberg, A. Weber-Bargioni. "Hyperspectral STS Mapping." *Methods and Applications of Autonomous Experimentation. in progress*

## Thesis

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

## Presentations

### Invited

1. "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).
2. "Machine Learning in Scanning Probe Microscopy." **J. C. Thomas**. Berkeley Lab's Energy Sciences Area, Science Hour, Lawrence Berkeley National Laboratory (2021).

### Contributed

1. "Transition Metal Dichalcogenide Defect Functionalization with Magnetic Impurities – Defect Introduction and Identification." **J. C. Thomas**. MRS Spring Meeting (2022).
2. "Scanning Probe Characterization over Defective WS<sub>2</sub> and 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 (2022).
3. "Machine-Driven Characterization and Classification over Au and WS<sub>2</sub>." **J. C. Thomas**. Machine Learning and Automated Experiment in Scanning Probe Microscopy, Virtual School, Oak Ridge National Laboratory (2021).
4. "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).
5. "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).
6. "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. "Defect Engineering within Transition Metal Dichalcogenides and Machine Learning Approaches towards STM/STS Tip Shaping on Au." **J. C. Thomas**, K. A. Cochrane, A. Weber-Bargioni. Graphene, Virtual (2020).
2. "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).
3. "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).
4. "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).
5. "Probing the Buried and Exposed Interface within Two-Dimensional Structures." **J. C. Thomas**, P. S. Weiss. Glenn T. Seaborg Symposium, UCLA (2013).
6. "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).
7. "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).
8. "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).

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## 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).

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## Mentoring & Outreach

- 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.

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## Affiliations

American Chemical Society

American Vacuum Society  
Materials Research Society  
American Physical Society  
Molecular Foundry  
California NanoSystems Institute  
NPJ Computational Materials - Journal Referee  
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, 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

Languages Python, C/C++, Java, SQL, JMP, Matlab

Frameworks PyTorch

WebDev HTML/CSS, JavaScript, PHP

Utilities Git, Jupyter Notebook

Graphics POV-Ray, Adobe, Blender

Communication English

## Awards

2021-ongoing 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

**Alexander Weber-Bargioni**  
*Staff Scientist*  
Molecular Foundry, LBNL  
afweber-bargioni@lbl.gov

**Marcus Noack**  
*Research Scientist*  
CAMERA, LBNL  
MarcusNoack@lbl.gov

**Paul S. Weiss**  
*Distinguished Professor*  
University of California, Los Angeles  
psw@cnsi.ucla.edu