

# John C. Thomas

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## Experience

- Sept 2024–ongoing **Senior Scientific Engineering Associate** LAWRENCE BERKELEY NATIONAL LABORATORY  
Advanced Light Source.  
  - Photon Science Development Group.
  - Instrumentation and projects.
  - Technical lead for cryogenic synchrotron infrared nano-spectroscopy.
  - Design, build, and implement experimental apparatus coupled to synchrotron photons.
- Oct 2023–Aug 2024 **Group Leader, Research Associate** DARTMOUTH COLLEGE  
Lawrence Berkeley National Laboratory & Thayer College of Engineering.  
  - Quantum low-temperature scanning probe group lead.
  - Independent research scientist focused on low-dimensional materials, scanning probe microscopy, and quantum defects.
  - Employed through Dartmouth College with work performed at Lawrence Berkeley National Laboratory.
- Mar 2020–Sept 2023 **Postdoctoral Fellow**, LAWRENCE BERKELEY NATIONAL LABORATORY  
Molecular Foundry & Materials Science Division.  
  - 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.
  - Execute user projects from collaborators across local and international institutions.
  - Train users for experiments on the SPM with a quantum science focus.
  - Implement tool automation and lead web development.
  - Maintain github libraries required for SPM experimental workflows, data analysis software development kits, and applied machine learning.
  - Design and implementation of free-space optics.
  - Thin-film material growth and characterization with numerous tool sets within the Molecular Foundry.
  - Scanning probe activity manager and safety lead.
- Dec 2018–Feb 2020 **Software Developer**, VERITOMYX, INC  
SDK developer.  
  - Implement API integration functionality within software development kits (SDKs) for mass spectrometer analytics and customer platform.
  - Contribute towards software solutions and systems design.
- Sep 2015–Nov 2018 **Process Technology & Development Engineer**, INTEL CORPORATION  
Defect metrology & yield analysis.  
  - Inline and end of line monitoring of silicon processes for HPC and SRAM, aimed at maximizing yield and reducing defectivity at multiple steps.
  - Trained and used statistical methods & design of experiments in tasks requested.

## Education

- 2015 **University of California, Los Angeles**  
*Physical Chemistry* Ph.D  
Department of Chemistry & Biochemistry  
California NanoSystems Institute
- 2008 **University of Texas at San Antonio**  
*Chemistry* B.S.  
Department of Chemistry

## Research Interests

**Instrumentation Design:** Design, fabrication, and assembly of scientific apparatus for measurements near or beyond the diffraction limit that couple in radio frequency (RF), magnetic (B) field, and high numerical aperture (NA) optical access.

**Optics:** Development of an optical system tailored for Fourier-transform infrared (FTIR) scattering-type scanning near-field optical microscopy (sSNOM). Optimized for sub-wavelength spatial resolution of chemical, structural, and electronic properties in materials.

**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** & A. Rossi, J. T. Kuchle, 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. "Graphene-driven correlated electronic states in one dimensional defects within WS<sub>2</sub>." *Nature Communications* **16**, 5809 (2025).
2. J. Liang, K. Ma, E. Walker, C. Johnson, X. Zhao, T. Terlier, **J. C. Thomas**, J. Wan, N. Dale, E. Rotenberg, A. Bostwick, C. Jozwiak, J.-W. Jang, M. Salmeron, P. D. Ashby, J. Kim, H. Zheng, A. Weber-Bargioni, T. Beechem, M. P. Sherburne, Z. Y. Al Balushi. "Spatially enhanced electrostatic doping in graphene realized via heterointerfacial precipitated metals." *Small* **21**, 2412750 (2025).
3. K. Nisi, **J. C. Thomas**, S. Levashov, E. Mitterreiter, T. Taniguchi, K. Watanabe, S. Aloni, T. R. Kuykendall, J. Eichhorn, A. W. Holleitner, A. Weber-Bargioni, C. Kastl. "Scanning probe spectroscopy of sulfur vacancies and MoS<sub>2</sub> monolayers in side-contacted van der Waals heterostructures." *2D Materials* **12**, 015023 (2024).
4. 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 Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene surfaces." *Matter* **7**, 2609 (2024).
5. **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 WS<sub>2</sub> discovered by high-throughput computational screening and fabricated by site-selective STM manipulation." *Nature Communications* **15**, 3556 (2024).
6. 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/ $\alpha$ -RuCl<sub>3</sub> Heterostructure via Angle-Resolved Photoemission Spectroscopy." *Nano Letters* **23**, 8000 (2023).
7. 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 WSe<sub>2</sub>." *Nano Letters* **23**, 4901 (2023).
8. **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).
9. 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).
10. **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).
11. **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).
12. 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).
13. **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).
14. **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).
15. J. N. Hohman, **J. C. Thomas**, Y. Zhao, H. Auluck, M. Kim, W. Vajselaar, 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).
16. 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).
17. 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).
18. 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).

## Journal Articles - Cont'd

19. 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).
20. J. N. Hohman, M. Kim, B. Schüpbach, M. Kind, **J. C. Thomas**, A. Terfort, and P. S. Weiss. "The Dynamic Double Lattice of 1-Adamantaneslenolate Self-Assembled Monolayers on Au{111}." *Journal of the American Chemical Society* **133**, 19422 (2011).
21. **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).
22. 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. W. Chen, **J. C. Thomas**, Y. Xiong, Z. Yu, D. Zhou, S. Kumari, Z. Dai, J. A. Robinson, M. Terrones, A. Raja, S. Griffin, A. Weber-Bargioni, G. Hautier. "First-Principles and experimental co-investigation of sulfur divacancy and nearest neighbor vacancy complexes in monolayer WS<sub>2</sub>." *in preparation*.
2. J. Zhou, **J. C. Thomas**, T. P. Darlington, E. S. Barnard, A. Taguchi, A. Schwartzberg, A. Weber-Bargioni. "Probing and Tuning Strain-Localized Exciton Emission in 2D Material Bubbles at Room Temperature." *in preparation*.

## 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." University of California, Los Angeles (2015). [link](#)

## Presentations

### Invited

1. "Identifying Quantum Defects at Relevant Length Scales: Experimental and Computational Investigations." **J. C. Thomas**. The Community for Autonomous Scientific Experimentation, Berkeley, CA, USA (2025).
2. "2D Material Quantum Defect Discovery: Autonomous Experimentation Combined with First-Principles Screening." **J. C. Thomas**. Computational Microscopy Conference, Lake Arrowhead, CA, USA (2024).
3. "Controlling Quasiparticle Excitations in 2D Solids Through Atomically Precise Heterostructures." **J. C. Thomas**. MRS Fall Meeting, Boston, MA (2023).
4. "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).
5. "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).
6. "Machine Learning in Scanning Probe Microscopy." **J. C. Thomas**. Berkeley Lab's Energy Sciences Area, Science Hour, Lawrence Berkeley National Laboratory (2021).

## Selected Contributed

1. "Quantum Defect Candidates at Modified Substitution Sites within WS<sub>2</sub>." **J. C. Thomas**. MRS Fall Meeting, Boston, MA (2023).
2. "Band gap renormalization across 1D mirror twin boundaries in WS<sub>2</sub>." **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<sub>2</sub>." **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<sub>2</sub>." **J. C. Thomas**. APS March Meeting, Las Vegas, NV (2023).
7. "Hyperspectral Scanning Tunneling Spectroscopy over WS<sub>2</sub> and 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<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, Chicago, IL (2022).
10. "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).
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).

## Selected Posters

1. "Quantum Defects by Design in 2D Materials." **J. C. Thomas**, G. Hautier, A. Weber-Bargioni. Molecular Foundry User Meeting, Berkeley, CA, USA (2023).
2. "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).
3. "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).
4. "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).
5. "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).

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## Mentoring & Outreach

2022- **Berkeley Lab Mentor**

Ongoing 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.

2023 **Organizer**

Quantum Information Science Winter School

Co-organized a Winter School for Quantum Information Science with colleagues from UC Berkeley, LBNL, LMU, TUM, and Max Planck for Quantum Optics in Munich.

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.

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## Affiliations

Advanced Light Source

Materials Research Society

American Physical Society

American Society of Precision Engineering

American Chemical Society

American Vacuum Society

Molecular Foundry

Center for Advanced Mathematics for Energy Research Applications (CAMERA)

Quantum Systems Accelerator (QSA)

Journal referee for numerous journals including: npj Computational Materials, Communications Physics, Nature Communications, Nature Materials, Small Structures, and others.

## Software

2022-2024 **Principal Developer of gpSTS**

Lawrence Berkeley National Laboratory.

2018-2020 **Developer on PeakInvestigator Project**

Veritomyx, Inc.

## Databases

2024 **Contributor to Quantum Defect Genome**

Lawrence Berkeley National Laboratory.

Dartmouth College.

## Certifications

2025 **Getting Started with Structural Analysis in Ansys Mechanical**

Ansys

2024 **Creo Analysis Professional Certification**

PTC University

2024 **Creo Associate Certification**

PTC University

2020 **Object Oriented Java Programming: Data Structures and Beyond**

Coursera

2019 **Applied Data Science with Python**

Coursera

## Skills

**Techniques** Scientific instrument design and operation, finite element analysis, scanning probe microscopy, optical spectroscopy, photoelectron spectroscopy, infrared spectroscopy, transmission and scanning electron microscopies, physical evaporation, low-energy electron diffraction, thin-film material growth, machine shop, clean room, and others.

**Languages** Python, C/C++, Java, SQL, JMP, LabVIEW, Matlab, Perl

**Frameworks** PyTorch, gpCAM, pymatgen, Windchill

**WebDev** HTML/CSS, JavaScript, PHP

**Utility** Git, Jupyter Notebook

**Graphics** POV-Ray, Adobe, Blender

**Application** Creo, Ansys Mechanical, SolidWorks, AutoCAD, VASP

**Language** English

## Awards

2023 **SPOT Award**

Lawrence Berkeley National Laboratory

2021-2022 **Energy Frontier Research Center Post Doctoral Fellowship**

Lawrence Berkeley National Laboratory