

## Curriculum Vitae

Liang Zheng Tan

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### Education

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<b>Ph.D. in Physics,</b> University of California, Berkeley, CA, USA Thesis supervisor: Prof. Steven G. Louie Dissertation: Electronic and vibrational properties of 2D materials constructed from graphene and molecular components	2008 – 2014
<b>B.Sc. in Physics,</b> California Institute of Technology, Pasadena, CA, USA	2005 – 2008

### Research Positions

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<b>Staff Scientist</b> Molecular Foundry, Lawrence Berkeley National Lab	2018-present
<b>Postdoctoral Fellow,</b> Department of Chemistry, University of Pennsylvania Supervisor: Prof. Andrew M. Rappe	2014-2018
<b>Graduate Student Researcher,</b> Dept. of Physics, University of California, Berkeley, and Material Sciences Division, Lawrence Berkeley National Lab	2009 - 2014
<b>Summer Undergraduate Research Fellowship,</b> Department of Physics, California Institute of Technology Advisor: Prof. John Preskill	2007 - 2008

### Awards

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<b>Graduate Division Summer Grant</b> Graduate Division, University of California, Berkeley	2012
<b>Berkeley Fellowship</b> Graduate Division, University of California, Berkeley	2008
<b>Summer Undergraduate Research Fellowship</b>	2007

Undergraduate research program, California Institute of Technology

**Richard G. Brewer Prize in Physics**

2006

Undergraduate Research Prize, California Institute of Technology

## Publications

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### *Manuscripts under review*

3. Upper limit on nonlinear optical processes: shift current and second harmonic generation in extended systems  
**LZ Tan** and AM Rappe  
arXiv:1708.05433 (2017)
2. Dynamic structural motions generate long-lived photo-excited polarization anisotropy in hybrid perovskites  
JPH Rivett, **LZ Tan**, MB Price, NJLK Davis, R Middleton, AM Rappe, D Credgington, F Deschler
1. Enhancing ferroelectric photovoltaic effect by polar order engineering  
L You, F Zheng, L Feng, Y Zhou, **LZ Tan**, Z Zhang, G Ma, D Schmidt, A Rusydi, L Wang, L Chang, AM Rappe, J Wang

### *Peer-reviewed journal articles*

orcid: <https://orcid.org/0000-0003-4724-6369>

27. Molecule-adsorbed topological insulator and metal surfaces: a comparative first principles study  
S Sarkar, J Yang, **LZ Tan**, AM Rappe and L Kronik  
*Chem. Mater.* 30, 1849-1855 (2018)  
<http://dx.doi.org/10.1021/acs.chemmater.7b03176>
26. Spin-orbit enhanced carrier lifetimes in noncentrosymmetric semiconductors  
**LZ Tan** and AM Rappe  
*J. Phys. Chem. Sol.* article ASAP (2018)  
<https://doi.org/10.1016/j.jpcs.2018.02.016>
25. Hybrid functional pseudopotentials  
J Yang, **LZ Tan** and AM Rappe  
*Phys. Rev. B* 97, 085130 (2018)  
<https://doi.org/10.1103/PhysRevB.97.085130>

24. Polarized emission in II-IV and perovskite colloidal quantum dots

M Isarov, **LZ Tan**, J Tilchin, F Rabouw, M Bodnarchuk, R van Dijk-Moes, R Carmi, Y Barak, A Kostadinov, I Meir, D Vanmaekelbergh, M Kovalenko, AM Rappe, E Lifshitz

*J. Phys. B: At. Mol. Opt. Phys.*, 50, 214001 (2017)

<https://doi.org/10.1088/1361-6455/aa8dd4>

23. Synthesis and physical properties of phase-engineered transition metal dichalcogenide monolayer heterostructures

CH Naylor, WM Parkin, Z Gao, J Berry, S Zhou, Q Zhang, JB McClimon, **LZ Tan**, CE Kehayias, M-Q Zhao, RS Gona, RW Carpick, AM Rappe, DJ Srolovitz, M Drndic, ATC Johnson

*ACS Nano*, **11**, 8619-8627 (2017)

<https://doi.org/10.1021/acsnano.7b03828>

22. Light-induced picosecond rotational disordering of the inorganic sublattice in the hybrid perovskites

X Wu, **LZ Tan**, X Shen, T Hu, K Miyata, MT Trinh, R Li, R Coffee, S Liu, DA Egger, I Makasyuk, Q Zheng, A Fry, JS Robinson, MD Smith, B Guzelturk, HI Karunadasa, X Wang, XY Zhu, L Kronik, AM Rappe, AM Lindenberg

*Science Advances* **3**, e1602388 (2017)

<https://doi.org/10.1126/sciadv.1602388>

21. Rashba effect in a single colloidal CsPbBr<sub>3</sub> perovskite nanocrystal detected by magneto-optical measurements

M Isarov, **LZ Tan**, MI Bodnarchuk, MV Kovalenko, AM Rappe, E Lifshitz

*Nano Lett.* **17**, 5020-5026 (2017)

<https://doi.org/10.1021/acs.nanolett.7b02248>

20. Large-area synthesis of high-quality monolayer 1T'-WTe<sub>2</sub> flakes

CH Naylor, WM Parkin, Z Gao, H Kang, M Noyan, RB Wexler, **LZ Tan**, Y Kim, CE Kehayias, F Streller, YR Zhou, R Carpick, Z Luo, YW Park, AM Rappe, M Drndic, JM Kikkawa, ATC Johnson

*2D Materials* **4**, 021008 (2017)

<https://doi.org/10.1088/2053-1583/aa5921>

19. Intermolecular Interactions in Hybrid Perovskites Understood from a Combined Density Functional Theory and Effective Hamiltonian Approach

**LZ Tan**, F Zheng, AM Rappe

*ACS Energy Lett.* **2**, 937-942 (2017)

<http://dx.doi.org/10.1021/acsenerylett.7b00159>

18. Local Polar Fluctuations in Lead Halide Perovskite Crystals

O Yaffe, Y Guo, **LZ Tan**, DA Egger, T Hull, C Stoumpos, F Zheng, TF Heinz, L Kronik, MG Kanatzidis, JS Owen, AM Rappe, MA Pimenta, LE Brus

*Phys. Rev. Lett.* **118**, 136001 (2017)

<https://doi.org/10.1103/physrevlett.118.136001>

17. Effective mass in bilayer graphene at low carrier densities: The role of potential disorder and electron-electron interaction

J Li, **LZ Tan**, K Zou, AA Stabile, DJ Seiwel, K Watanabe, T Taniguchi, SG Louie, J Zhu

*Phys. Rev. B* **94**, 161406 (2016)

<https://doi.org/10.1103/PhysRevB.94.161406>

16. Shift Current Bulk Photovoltaic Effect in Polar Materials - hybrid and oxide perovskites and beyond

**LZ Tan**, F Zheng, SM Young, F Wang, S Liu, AM Rappe

*npj Comput. Mat.* **2**, 16026 (2016)

<http://dx.doi.org/10.1038/npjcompumats.2016.26>

15. High Chloride Doping Levels Stabilize the Perovskite Phase of Cesium Lead Iodide

S Dastidar, DA Egger, **LZ Tan**, SB Cromer, AD Dillon, S Liu, L Kronik, AM Rappe, AT Fafarman

*Nano Lett.* **16** (6), 3563-3570 (2016)

<https://doi.org/10.1021/acs.nanolett.6b00635>

14. Enhancement of Bulk Photovoltaic Effect in Topological Insulators

**LZ Tan**, AM Rappe

*Phys. Rev. Lett.* **116**, 237402 (2016)

<https://doi.org/10.1103/PhysRevLett.116.237402>

13. Strain-Induced Ferroelectric Topological Insulator

S Liu, Y Kim, **LZ Tan**, AM Rappe

*Nano Lett.* **16** (3), 1663-1668 (2016)

<https://doi.org/10.1021/acs.nanolett.5b04545>

12. Rashba Spin-Orbit Coupling Enhanced Carrier Lifetime in  $\text{CH}_3\text{NH}_3\text{PbI}_3$

F Zheng, **LZ Tan**, S Liu, AM Rappe

*Nano Lett.* **15** (12), 7794-7800 (2015)

<https://doi.org/10.1021/acs.nanolett.5b01854>

11.  $\text{SU}(4)$  symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene

**LZ Tan**, M Orlita, M Potemski, J Palmer, C Berger, WA de Heer, SG Louie, G Martinez

*Phys. Rev. B* **91**, 235122(2015)

<https://doi.org/10.1103/PhysRevB.91.235122>

10. Manipulation and characterization of aperiodical graphene structures created in a two-dimensional electron gas

S. Wang, **LZ Tan**, W. Wang, S. G. Louie, and N. Lin

*Phys. Rev. Lett.* **113**, 196803 (2014)

<https://doi.org/10.1103/PhysRevLett.113.196803>

9. Imaging and Tuning Molecular Levels at the Surface of a Gated Graphene Device

A. Riss, S. Wickenburg, **LZ Tan**, H.-Z. Tsai, Y. Kim, J. Lu, A. J. Bradley, M. M. Ugeda, K. L. Meaker, K. Watanabe, T. Taniguchi, A. Zettl, F. R. Fischer, S. G. Louie, M. F. Crommie

*ACS Nano* **8** (6), pp 5395 (2014)

<https://doi.org/10.1021/nn501459v>

8. Local electronic and chemical structure of Oligo-Acetylene Derivatives Formed through radical cyclizations at a surface

A. Riss, S. Wickenburg, P. Gorman, **LZ Tan**, H.-Z. Tsai, D. G. de Oyteza, Y. C. Chen, A. J. Bradley, M. M. Ugeda, G. Etkin, S.G. Louie, F. R. Fischer, M. F. Crommie

*Nano Lett.* **14** (5), pp 2251 (2014)

<https://doi.org/10.1021/nl403791q>

7. Tuning two-dimensional band structure of Cu(111) surface-state electrons interplayed with artificial supramolecular architectures

S. Wang, W. Wang, **LZ Tan**, X. G. Li, P. N. Liu, S. G. Louie, N. Lin

*Phys. Rev. B* **88**, 245430 (2013)

<https://doi.org/10.1103/PhysRevB.88.245430>

6. Theory of the Raman spectrum of rotated double-layer graphene

S. Coh, **LZ Tan**, S. G. Louie, and M. L. Cohen

*Phys. Rev. B* **88**, 165431 (2013)

<https://doi.org/10.1103/PhysRevB.88.165431>

5. Raman Spectroscopy Study of Rotated Double-Layer Graphene: Misorientation-Angle Dependence of Electronic Structure

K. Kim, S. Coh, **LZ Tan**, W. Regan, J. M. Yuk, E. Chatterjee, M. F. Crommie, M. L. Cohen, S. G. Louie, A. Zettl

*Phys. Rev. Lett.* **108**, 246103 (2012)

<https://doi.org/10.1103/PhysRevLett.108.246103>

4. Resonant Excitation of Graphene K-Phonon and Intra-Landau-Level Excitons in Magneto-Optical Spectroscopy

M. Orlita, **LZ Tan**, M. Potemski, M. Sprinkle, C. Berger, W. A. de Heer, S. G. Louie, G. Martinez

*Phys. Rev. Lett.* **108**, 247401 (2012)

<https://doi.org/10.1103/PhysRevLett.108.247401>

3. New Dirac Fermions in Periodically Modulated Bilayer Graphene

**LZ Tan**, C.-H. Park, and S. G. Louie

*Nano Lett.* **11** (7), pp 2596–2600 (2011)

<https://doi.org/10.1021/nl200055s>

2. Theory of the electronic and transport properties of graphene under a periodic electric or magnetic field

C.-H. Park, **LZ Tan**, S. G. Louie

*Physica. E, Low-dimensional systems & nanostructures* **43**, 651 (2011)

<https://doi.org/10.1016/j.physe.2010.07.022>

1. Graphene Dirac fermions in one-dimensional inhomogeneous field profiles: Transforming magnetic to electric field

**LZ Tan**, C.-H. Park, and S. G. Louie

*Phys. Rev. B* **81**, 195426 (2010)

<https://doi.org/10.1103/PhysRevB.81.195426>

#### *Book Chapters*

1. Ferroelectricity and spin-orbit coupling in organic-inorganic perovskite halides

DD Sante, A Stroppa, **LZ Tan**, P Barone, AM Rappe, S Picozzi

*Theoretical modeling of organohalide perovskites for photovoltaic applications*, Ed. G Giogi, K Yamashita (2017)

#### Conference Presentations

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##### *Invited talks*

4. “Coupled optical-electronic-vibrational motions in lead halide perovskites”

Computer simulation studies in condensed matter physics, Workshop at University of Georgia, 2018

3. “Rashba effect on the photophysical properties of hybrid perovskites and topological insulators”

SPIE Nanoscience+Engineering, 2017, San Diego, CA

2. “Optics and photo-physics of hybrid perovskites reveals via multi-scale modeling”

SPIE Nanoscience+Engineering, 2017, San Diego, CA

1. “Structure and electronic structure of halide perovskites from first-principles”

Electronic and structural dynamics in hybrid perovskites: theory meets experiment, 2016, Telluride, CO

##### *Contributed talks*

16. “Upper limit on nonlinear optical processes: shift current and second harmonic generation in extended systems”

New Horizons in Photovoltaics Symposium 2017, Philadelphia, PA

15. “Local polar fluctuations in lead halide perovskites”  
American Physical Society (APS) March Meeting 2017, New Orleans, LA
14. “Hybrid functional pseudopotentials”  
American Chemical Society (ACS) Spring meeting 2017, San Francisco, CA
13. “Nature of dynamic disorder in lead-halide perovskite photovoltaics”  
American Chemical Society (ACS) Fall meeting 2016, Philadelphia, PA
12. “Enhancement of bulk photovoltaic effect in layered topological insulator BiTeI”  
American Physical Society (APS) March Meeting 2016, Baltimore, MD
11. “Extensive first-principles study of the energy landscape of hybrid organometallic perovskites”  
American Chemical Society (ACS) Spring meeting 2016, San Diego, CA
10. “Layered 2D carbon: theory and applications of graphene nanostructures”  
World Congress of Smart Materials, 2016, Singapore
9. “Understanding molecular orientational disorder in the hybrid perovskites: interplay of hydrogen bonding and PbI<sub>3</sub> lattice distortions”  
Fundamental Physics of Ferroelectrics and related materials 2016, Washington, DC
8. “SU(4) symmetry breaking revealed by magneto-optical spectroscopy in epitaxial graphene”  
American Physical Society (APS) March Meeting 2015, San Antonio, TX
7. “Two-dimensional topological insulator molecular networks: dependence on structure, symmetry, and composition”  
American Physical Society (APS) March Meeting 2014, Denver, CO
6. “Optimizing the design of artificial lattices”  
American Physical Society (APS) March Meeting 2013, Baltimore, MD
5. “Optimizing the design of artificial graphene”  
Seminar at Laboratoire National des Champs Magnetiques Intenses, CNRS, Grenoble, France, September 2012
4. “Band mass renormalization in bilayer graphene – ab initio GW calculations”  
International Conference of Young Researchers on Advanced Materials, Singapore, July 2012
3. “Electron-hole asymmetry and band mass renormalization in bilayer graphene: elucidating the role of electron-electron interactions with first-principles GW calculations”  
American Physical Society (APS) March Meeting 2012, Boston, MA
2. “Landau level-phonon resonances in graphene and their spectroscopic signatures in magneto-optical measurements”  
American Physical Society (APS) March meeting 2011, Dallas, TX

1. “Carrier velocity reduction in magnetic graphene superlattices”  
American Physical Society (APS) March Meeting 2010, Portland, OR

#### *Poster presentations*

5. “Materials design for shift current bulk photovoltaic effect”, New Horizons in Photovoltaics Symposium, 2017, Philadelphia, PA
4. “Pushing nonlinear spectroscopy to its limit: Theoretical upper bounds for second harmonic generation in molecules and materials”, American Chemical Society (ACS) Fall meeting, Academic Employment Initiative, 2017, Washington, DC
3. “Spin-orbit coupling enhanced carrier lifetimes in organometal halide perovskites”, Materials Research Society Fall meeting, 2015, Boston, MA
2. “Enhancing the bulk photovoltaic effect using topology”, New Vistas in Photovoltaics Symposium, 2015, Philadelphia, PA
1. “Bulk photovoltaic effect in topological insulators”, Penn Conference in Theoretical Chemistry 2015, Philadelphia, PA

### Teaching and Mentoring

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#### *University teaching experience*

**Instructor,** Fall 2017  
MSE 360 Structure at the Nanoscale – Crystallography and diffraction for upperclassmen  
Department of Materials Science and Engineering, University of Pennsylvania  
Taught biweekly lectures, designed curriculum, developed exams and assignments, and supervised teaching assistants

**Teaching Assistant,** 2012-2013  
Physics 240 – Graduate level solid state physics (Prof. Steven G. Louie)  
Department of Physics, University of California at Berkeley  
Led recitation sections, graded assignments and exams

**Teaching Assistant,** Spring 2008  
Physics 8b – Introductory electricity and magnetism for freshmen (Prof. Mike DeWeese)  
Department of Physics, University of California at Berkeley  
Led recitation sections and labs, graded assignments and exams

#### *Mentorship of students*

During my postdoctoral appointment, I supervised four graduate students and two undergraduate students in framing and developing their research projects, in the running



of first-principles density functional theory calculations, and in the writing of research papers.

## Service

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### **Reviewer**

2014-present

Reviewed manuscripts for: Nature Communications; Nanoscale; Physical Review B; Journal of Applied Physics; Solid State Communications;

### **Preliminary exam committee**

(2009)

University of California at Berkeley

Vetted prelim exam questions for incoming graduate students