Diana Y. Qiu

Assistant Professor
Department of Mechanical Engineering and Materials Science
Yale University

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Employment

Assistant Professor, 2020-present, Yale University, New Haven, CT, USA
- Primary appointment: Mechanical Engineering and Materials Science
- Courtesy appointments: Physics, Applied Physics

Postdoctoral Researcher, 2017-2019, Lawrence Berkeley National Lab, Berkeley, CA, USA

Education

Ph.D. Physics, University of California, Berkeley, August 2017
- Advisor: Prof. Steven G. Louie
- Thesis: Many-Body Effects on the Quasiparticle and Optical Properties of Quasi-two-dimensional Systems

B.S. Physics, Yale University, May 2011

Awards and Honors

National Academy of Sciences Kavli Fellow, 2024
NSF Career Award, 2023
Packard Fellowship for Science and Engineering, 2021
DOE Early Career Award, 2021
Rising Stars in Physics Workshop, Massachusetts Institute of Technology, 2018
Jackson C. Koo Award, 2017
National Science Foundation Graduate Research Fellowship, 2011-2016
Berkeley Chancellor's Fellowship, 2011-2013
Howard L. Schultz Prize, 2011
Barry Goldwater Scholarship, 2010

All Journal Publications

(Publication Metrics from Google Scholar: Published 53 articles, cited 7,000+ times, h-index=25)
*=corresponding author (last author unless otherwise noted)
†=equal contribution

1. A.M. Alvertis, A. Champagne, M. Del Ben, F.H. da Jornada, D.Y. Qiu, M.R. Filip, J.B. Neaton, "Importance of nonuniform Brillouin zone sampling for first-principles calculations of exciton binding energies in semiconductors and insulators," *Physical Review B* **108**, 235117 (2023).

2. S. Stolz, D. Wang, B. Hou, A. Kozhakhmetov, C. Dong, O. Groning, J.A. Robinson, **D.Y. Qiu**, B, Schuler, "Spin-stabilization by Coulomb blockade in a vanadium dimer in WSe2," accepted in *ACS Nano* (2023).
3. M. Gu*, Y. Lin, V. Chang Lee, **D.Y. Qiu*,** "Probabilistic forecast of nonlinear dynamical systems with uncertainty quantification," *Physica D: Nonlinear Phenomena*, 457, 133938 (2023).
4. J.B. Haber, **D.Y. Qiu**, F.H. da Jornada, J.B. Neaton, "Maximally-localized Wannier functions for excitons in solids", accepted in *Physical Review B* (2023).
5. Y.H. Chan*, **D.Y. Qiu***, F.H. da Jornada*, S.G. Louie*, "Giant self-driven exciton-Floquet signatures in time-resolved photoemission spectroscopy of MoS2 from time-dependent GW approach," accepted in *Proceedings of the National Academy of Science* (2023).
6. B. Hou, D. Wang, B. A. Barker, **D. Y. Qiu**, "Intermixing of Bulk and Topological Surface State by Chiral Excitons in Bi_2Se_3," *Physical Review Letters*, 130, 206402 (2023).
7. J. McArthur, M. R. Filip, **D. Y. Qiu**, "Minimal Molecular Building Blocks for Screening in Quasi-Two-Dimensional Organic–Inorganic Lead-Halide Perovskites," *Nano Letters*, 23, 3796-3902 (2023).
8. Y.-H. Chan*, J. B. Haber, M. H. Naik, J. B. Neaton, **D. Y. Qiu***, Felipe H. da Jornada*, Steven G. Louie*, "Exciton lifetime and optical linewidth profile via exciton-phonon interactions: Theory and first-principles calculations for monolayer MoS_2," *Nano Letters*, 23, 3971-3977 (2023).
9. A. Champagne, J .B. Haber, S. Pokawanvit, **D. Y. Qiu**, S. Biswas, H. A. Atwater, F.H. da Jornada, J.B. Neaton, "Quasiparticle and Optical Properties of Carrier-Doped Monolayer MoTe2 from First Principles," *Nano Letters*, 23, 4274-4281 (2023).
10. S. Biswas, A. Champagne, J. B. Haber, S. Pokawanvit, J. Wong, H. Akbari, S. Krylyuk, K. Watanabe, T. Taniguchi, A. V. Davydov, Z. Y. Al Balushi, **D. Y. Qiu**, F. H. da Jornada, J. B. Neaton, H. A. Atwater, "Rydberg Excitons in Monolayer $MoTe_2$," *ACS Nano*, 17, 7685–7694 (2023).
11. J. Yin, Y. Chan, F. da Jornada, **D. Y. Qiu**, C. Yang, S.G. Louie, "Analyzing and predicting non-equilibrium many-body dynamics via dynamic mode decomposition," *Journal of Computational Physics*, 477, 11909 (2023).
12. T. Amit, D. Hernangómez-Pérez, G. Cohen, **D. Y. Qiu**, S. Refaely-Abramson, "Tunable magneto-optical properties in MoS2 via defect-induced exciton transitions," *Physical Review B*, 106, L161407 (2022).
13. L. Yue, R. Hollinger, C.B. Uzundal, B. Nebgen, Z. Gan, A. George, C. Spielmann, D. Kartashov, A. Turchanin, **D.Y. Qiu**, M.B. Gaarde, M. Zuerch, "Signatures of multi-band effects in high-harmonic generation in monolayer MoS2," *Physical Review Letters*, 129, 147410 (2022).
14. J. Yin, Y. Chan, F. da Jornada, **D. Y. Qiu**, S.G. Louie, C. Yang, "Using Dynamic Model Decomposition to Predict the Dynamics of a Two-time Non-equilibrium Green's function," *Journal of Computational Science*, 64, 101843 (2022).
15. M.R. Filip, **D.Y. Qiu**, M. Del Ben and J.B. Neaton "Screening of Excitons by Organic Cations in Quasi-Two-Dimensional Organic–Inorganic Lead-Halide Perovskites." *Nano Letters*, 12, 4870–4878 (2022).
16. M. Wang, A. Kumar, H. Dong, J.M. Woods, J.V. Pondick, S. Xu, P. Guo, **D.Y. Qiu**, J.J. Cha, "A Gapped Phase in Semimetallic Td-WTe2 Induced by Lithium Intercalation." *Advanced Materials*, 220861 (2022).
17. F. Tang, Z. Li, C. Zhang, S.G. Louie*, R. Car*, **D.Y. Qiu***, X. Wu,* "Many-Body Effects in the X-ray Absorption Spectra of Liquid Water," *Proceedings of the National Academy of Sciences*, 119, e2201258119 (2022).
18. P. Wang, W. Lee, P. Corbett, W.H. Koll, N.M. Vu, D.A. Laleyan, Q. Wen, Y. Wu, A. Pandely, J. Gim, D. Wang, **D.Y. Qiu**, R. Hovden, M. Kira, J.T. Heron, J.A. Gupta, A. Kioupakis, Z. Mi, "Scalable Synthesis of Monolayer Boron Nitride on Graphene," *Advanced Materials*, 2201387 (2022).
19. J.V. Pondick, S. Yazdani, A. Kumar, D. J. Hyneck. J.L. Hart, M. Wang, **D.Y. Qiu**, J.J. Cha, "Thickness-dependent phase transition kinetics in lithium-intercalated MoS_2," *2D Materials*, 9, 025009 (2022).
20. **D.Y. Qiu***, G. Cohen, D. Novichkova, S. Refaely-Abramson, "Signatures of Dimensionality and Symmetry in Exciton Bandstructure: Consequences for Time-Evolution," *Nano Letters* 21, 7644-7650 (2021).
21. J.V. Pondick, A. Kumar, M. Wang, S. Yazdani, J.M. Woods, **D.Y. Qiu**, J.J. Cha, "Heterointerface control over lithium-induced phase transitions in MoS2 nanosheets: implications for nanoscaled energy materials," *ACS Appl. Nano Mater*., 4, 14105-14114 (2021).
22. C. Zhang, F. Tang, M. Chen, J. Xu, L. Zhang, **D.Y. Qiu**, J.P. Perdew, M.L. Klein, X. Wu, "Modeling liquid water by climbing up Jacob's ladder in density functional theory facilitated by using deep neural network potentials," *J. Phys. Chem. B* 125, 11444-11456 (2021).

23. K.Q. Lin, C.S. Ong, S. Bange, P.E. Faria Jr, B. Peng, J.D. Ziegler, J. Zipfel, C. Bäuml, N. Paradiso, K. Watanabe, T. Taniguchi, C. Strunk, B. Monserrat, J. Fabian, A. Chernikov, **D. Y. Qiu**, S.G. Louie, J.M. Lupton, "Narrow-band transitions of high-lying excitons in monolayer WSe2," *Nature Communications*, 12, 5500 (2021).
24. F. Tang, J. Xu, **D.Y. Qiu***, X. Wu*, "Nuclear quantum effects on the quasiparticle properties of the chloride anion aqueous solution within the GW approximation," *Phys. Rev. B*, 104, 035117 (2021).
25. E. Mitterreiter, B. Schuler, A. Micevic, D. Hernangómez-Pérez, K. Barthelmi, K.A. Cochrane, J. Kiemle, F. Sigger, J. Klein, E. Wong, E.S. Barnard, K. Watanabe, T. Taniguchi, M. Lorke, F. Jahnke, J.J. Finley, A.M. Schwartzberg, S. Refaely-Abramson, **D.Y. Qiu**, A.W. Holleitner, A. Weber-Bargioni, C. Kastl, "The role of chalcogen vacancies for atomic defect emission in MoS2," *Nature Communications*, 12, 3822 (2021).
26. Y. H. Chan, **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie, "Giant exciton-enhanced shift currents and DC conduction with sub-bandgap photo excitations produced by many-electron interactions." *Proceedings of the National Academy of Sciences*, 118. (2021)
27. S. G. Louie*, Y.-H. Chan, F.H. da Jornada, Z.L. Li, **D.Y. Qiu**, "Discovering and understanding materials through computation. *Nature Materials*, 20, 728–735 (2021).
    Note: This is an invited Commentary.
28. H.M. Bretscher, Z. Li, J. Xiao, **D.Y. Qiu**, S. Refaely-Abramson, J. Alexander-Webber, A.O.A. Tanoh, Y. Fan, G. Delport, C. Williams, S.D. Stranks, S. Hofmann, J.B. Neaton, S. G. Louie, and A. Rao, "Rational Passivation of Sulfur Vacancy Defects in Two-Dimensional Transition Metal Dichalcogenides," *ACS Nano* (2021).
29. S. Yazdani, J.V. Pondick, A. Kumaar, M. Yarali, J.M. Woods, D.J. Hynek, **D.Y. Qiu**, J.J. Cha, "Heterointerface effects on lithium-induced phase transitions in intercalated MoS_2," *ACS Applied Material Interfaces*, 13 10603-10611 (2021).
30. S. Yoon, T. Kim, S. Seo, S.-H. Shin, S.-B. Song, B. J. Kim, K. Watanabe, T. Taniguchi, G.-H. Lee, M. Jo, **D. Y. Qiu***, J. Kim*, "Electrical control of anisotropic and tightly bound excitons in bilayer phosphorene," *Physical Review B*, 103, L041407 (2021).
31. **D. Y. Qiu**, F.H. da Jornada, S.G. Louie, "Solving the Bethe-Salpeter Equation on a Subspace: Approximations and Consequences for Low-dimensional Materials," *Physical Review B*, 103, 045117 (2021).
    Chosen as **Editor's Suggestion**.
32. **D.Y. Qiu,** S. Coh, M.L. Cohen, and S. G. Louie, "Comparison of GW band structure to semiempirical approach for an FeSe monolayer," Physical Review B, 101, 235154 (2020).
33. S. Barja†, S. Refaely-Abramson†, B. Schuler†, **D. Y. Qiu**†, A. Pulkin, S. Wickenburg, H. Ryu, M. M. Ugeda, C. Kastl, C. Chen, C. Hwang, A. Schwartzberg, S. Aloni, S.-K. Mo, D. F. Ogletree, M. F. Crommie, O. Yazyev, S. G. Louie, J. B. Neaton, and A. Weber-Bargioni, "Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides." *Nature Communications* 10, 1-8 (2019).
34. B. Schuler, **D. Y. Qiu**, S. Refaely-Abramson, C. Kastl, C.T. Chen, S. Barja, R.J. Koch, D.F. Ogletree, S. Aloni, A.M. Schwartzberg, S. G. Louie, J. B. Neaton, and A. Weber-Bargioni, "Large Spin-Orbit Splitting of Deep In-Gap Defect States of Engineered Sulfur Vacancies in Monolayer WS_2," *Physical Review Letters* 123, 07681 (2019).
    Chosen as **Editor's Suggestion**.
35. M.I.B. Utama, H. Kleemann, W. Zhao, C.S. Ong, F. H. da Jornada, **D. Y. Qiu**, H. Cai, H. Li, R. T. Kou, S. Zhao, S. Wang, K. Watanabe, T. Taniguchi, S. Tongay, A. Zettl, S. G. Louie, and F. Wang, "Dielectric-Defined Lateral Heterojunction in a Monolayer Semiconductor," *Nature Electronics*, 2, 60-65 (2019).
36. S. Refaely-Abramson†, **D. Y. Qiu**†, S. G. Louie, and J.B. Neaton, "Defect-induced modification of low-lying excitons and valley selectivity in monolayer transition metal dichalcogenides," *Physical Review Letters, 121, 167402* (2018).
37. G. Antonius, **D. Y. Qiu**, and S. G. Louie, "Orbital Symmetry and the Optical Response of Single-layer Monochalcogenides," *Nano Letters*, 18, 1925-1929 (2018)
38. A. Yan, C. S. Ong, **D. Y. Qiu**, C. Ohpus, J. Ciston, C. Merino, S. G. Louie, and A. Zettl, "Dynamics of Symmetry-Breaking Stacking Boundaries in MoS_2," *J. Phys. Chem. C*, 121, 22559-22566 (2017).
39. **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie, "Environmental Screening Effects in 2D Materials: Renormalization of the Bandgap, Electronic Structure, and Optical Spectra of Few-Layer Black-Phosphorus," *Nano Letters*, 17, 4706-4712 (2017).

40. F. H. da Jornada†, **D. Y. Qiu**†, and S. G. Louie, "Non-uniform sampling schemes of the Brillouin zone for many-electron perturbation-theory calculations in reduced dimensionality," *Physical Review B*, 95, 035109 (2017).
41. K. Hippalgaonkar, Y. Wang, Y. Ye, **D. Y. Qiu**, H. Zhu, Y. Wang, J. Moore, S.G. Louie, and X. Zhang, "High Thermoelectric Powerfactor in 2D Crystals of MoS_2," *Physical Review B*, 95, 115407 (2017).
42. L. Li, J. Kim, C. Jin, G. Ye, **D. Y. Qiu**, F. H. da Jornada, Z. Shi, L. Chen, Z. Zhang, F. Yang, K. Watanabe, T. Taniguchi, W. Ren, S. G Louie, X. Chen, Y. Zhang, and F. Wang, "Direct Observation of Layer-Dependent Electronic Structure in Phosphorene," *Nature Nanotechnology*, 12, 21-25 (2017).
43. T. Cao, Z. Li, **D. Y. Qiu**, and S. G. Louie, "Gate Switchable Transport and Optical Anisotropy in 90° Twisted Bilayer Black Phosphorus," *Nano Letters*, 16, 5542–5546 (2016).
44. **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie," Screening and many-body effects in two-dimensional crystals: Monolayer MoS_2," *Physical Review B*, 93, 235435 (2016).
45. D. P. Kumah, M. Dogan, J. H. Ngai, **D. Y. Qiu**, Z. Zhang, D. Su, E. D. Specht, S. Ismail-Beigi, C. H. Ahn, and F. J. Walker, "Engineered Unique Elastic Modes at a $BaTiO_3$/(2×1)−Ge(001) Interface," *Physical Review Letters*, 116, 106101 (2016).
46. **D. Y. Qiu**, T. Cao, and S. G. Louie, "Nonanalyticity, valley quantum phases, and lightlike exciton dispersion in monolayer transition metal dichalcogenides: Theory and first-principles calculations," *Physical Review Letters*, 115, 176801 (2015).
    Chosen as **Editor's Suggestion**.
47. A. J. Bradley, M. M. Ugeda, F. H. da Jornada, **D. Y. Qiu**, W. Ruan, W. Zhang, S. Wickenburg, A. Riss, J. Lu, S.-K. Mo, Z. Hussain, Z.-X. Shen, S. G Louie, and M. F. Crommie, "Probing the Role of Interlayer Coupling and Coulomb Interactions on Electronic Structure in Few-Layer $MoSe_2$ Nanostructures," *Nano Letters*, 15, 2594-2599 (2015).
48. Z. Zhou, M. Trassin, Y. Gao, Y. Gao, **D. Y. Qiu**, K. Ashraf, T. Nan, X. Yang, S. R Bowden, D. T. Pierce, M. D. Stiles, J Unguris, M. Liu, B. M Howe, G. J. Brown, S. Salahuddin, R. Ramesh, and N. X Sun, "Probing electric field control of magnetism using ferromagnetic resonance," *Nature Communications*, 6, 6082 (2015).
49. M. M. Ugeda, A. J. Bradley, S.-F. Shi, F. H. da Jornada, Y. Zhang, **D. Y. Qiu**, W. Ruan, S.-K. Mo, Z. Hussain, Z.-X. Shen, F. Wang, S. G. Louie, and M. F. Crommie , "Giant bandgap renormalization and excitonic effects in a monolayer transition metal dichalcogenide semiconductor," *Nature Materials*, 13, 1091-1095 (2014).
50. K. Liu, L. Zhang, T. Cao, C. Jin, **D. Y. Qiu**, Q. Zhou, A. Zettl, P. Yang, S. G. Louie, and F. Wang, "Evolution of interlayer coupling in twisted molybdenum disulfide bilayers," *Nature Communications*, 5, 4966 (2014).
51. **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie , "Optical spectrum of MoS_2: many-body effects and diversity of exciton states," *Physical Review Letters*, 111, 216805 (2013). Erratum: *Phys Rev Lett*, 115, 119901 (2015).
52. **D. Y. Qiu**, K. Ashraf, and S. Salahuddin , "Nature of magnetic domains in an exchange coupled BiFeO3/CoFe heterostructure," *Applied Physics Letters*, 102, 112902 (2013).
53. P.-O. Jubert, B. Biskeborn, **D. Y. Qiu**, A. Matsumoto, H. Noguchi, O. Shimizu , "Noise and recording properties of barium-ferrite particulate media studied by micromagnetic modeling," *IEEE Transactions on Magnetics*, 47, 386-394 (2011).

Submitted Publications & Pre-prints

1. G. Cohen, J. B. Haber, **D.Y. Qiu***, S. Rafaely-Abramson*, "Phonon-driven femtosecond dynamics of excitons in crystalline pentacene from first principles," under review at *Physical Review Letters*, arXiv:2305.04223v1 (2023).
2. V. Pareek, D. Bacon, X. Zhi, Y.-H. Chan, F. Bussolotti, N. S. Chan, J. P. Urquizo, K. Watanabe, T. Taniguchi, M. K. L. Man, J. Madéo, **D. Y. Qiu**, K. E. J. Goh, F. H. Jornada, K. M. Dani, "Driving Floquet physics with excitonic fields," under review at *Science* (2023).
3. S. Li†, X. Xu†, C.A. Kocoj, C. Zhou, Y. Li, D. Chen, J.A. Bennett, S. Liu, L. Quan, M. Liu, **D.Y. Qiu*,** P. Guo*, "Large exchange-driven intrinsic circular dichroism of a chiral 2D hybrid perovskite," under review at *Nature Communications* (2023).
4. V. Chang Lee, L. Yue, M.B. Gaarde, Y.-H. Chan, **D.Y. Qiu**, "Many-body enhancement of high harmonic generation in monolayer MoS_2," under review at *Nature Communications* (2023).

Reviewed Conference Proceedings

1. A. Guggenmos, H.-T. Chang, M. Zurch, **D. Y. Qiu**, R. Geneaux, C. H. Chen, X. Wei, C.M. Jiang, Y. Liang, F. H. da Jornada, A. Schwartzberg, D. Prendergast, V.C. Tung, S. G. Louie, D. M. Neumark, S. R. Leone, "Electron dynamics in transition metal dichalcogenides utilizing attosecond transient absorption spectroscopy," *CLEO: QELS_Fundamental Science*, FF1P.4 (2018).
2. R. Hollinger, L Yue, C. B. Uzundal, Z. Gan, A. George, C. Spielmann, D. Kartashov, A. Turchanin, **D. Y. Qiu**, M. B. Gaarde, M. Zuerch, "High harmonic generation anisotropy from a monolayer MoS2," *OSA Technical Digest*, NW2A.4, Optical Society of America (2021).

Current Grants & Funding

David and Lucile Packard Foundation Fellowship for Science and Engineering
- *Computation of Exciton Dynamics from First Principles*
- Role: sole PI
- Amount: $875,000
- Year: 2021-2026

DOE Early Career Research Program
- *First Principles Approach to Exciton Transport in Energy Materials*
- Role: sole PI
- Amount: $750,000
- Year: 2021-2026

NSF Condensed Matter and Materials Theory Program
- *Ab Initio Downfolding Approach to Dynamical Exciton-Continuum Interactions*
- Role: sole PI
- Amount: $363,725
- Year: 2021-2024

DOE Computational Materials Science Center
- *Center for the Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM)*
- Role: co-PI
- Amount: $600,000 (Yale sub-award)
- Year: 2020-2024

NSF National Research Traineeship Program
- *Interdisciplinary Graduate Program in Quantum Materials and Engineering at Yale*
- Role: senior personnel
- Amount: $3,000,000
- Year: 2023-2028

NSF Career Award
- *Real-Time First-Principles Approach to Understanding Many-Body Effects on High Harmonic Generation in Solids*
- Role: sole PI
- Amount: $675,000
- Year: 2024-2029

Past Grants and Funding

Yale Planetary Solutions Seed Project
- *A New Paradigm for Solar Energy Harvesting Based on the Bulk Photovoltaic Effect*
- Role: PI
- Amount: $80,000 ($26,666 allocated to PI)

- Year: 2022

Current Computation and Instrumentation Grants

DOE INCITE AWARD
- *Novel Methods for Complex Excited-State Phenomena in Functional Materials*
- Role: co-PI
- Amount: 400,000 GPU Node Hours (Summit)
- Year: 2023

DOE National Energy Research Scientific Computing Center (NERSC) Mission Science Award
- *Electronic and Optical Properties of Layered Materials for Energy Applications*Role: co-PI
- Role: PI
- Amount: 29,823 CPU Node Hours; 20,000 GPU Node Hours (Perlmutter)
- Year: 2023

NSF Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) Award
- *Investigation of two-dimensional materials for energy and optical applications using ab initio many-body perturbation theory*
- Role: PI
- Amount: 50,000 CPU Node Hours (Stampede); 2,060,238.0 SUs (Purdue Anvil)
- Year: 2022-2023

Texas Advanced Computing Center (TACC) Frontera Pathways Award
- *First-principles study of many-body interactions and excited-state properties in two-dimensional materials*
- Role: PI
- Amount: 225,000 CPU Node Hours (Frontera)
- Year: 2022-2023

DOE ASCR Leadership Computing Challenge (ALCC)
- *Dynamics and Decoherence of Excited States in 2D Systems for Quantum Technology*
- Role: co-PI
- Amount: 100,000 GPU Node Hours (Summit)
- Year: 2022-2023

Teaching

MENG 492/ENAS 755 Electronic and Optical Properties of Energy Materials, Yale University, Spring 2021, Spring 2023, Spring 2024
- Course director
- Number of Lectures: 25
- Contact hours: ~4 hours/week
- Enrollment: 9

MENG 280 Strength and Deformation of Mechanical Elements, Yale University, Fall 2021, Fall 2022, Fall 2023
- Course director
- Number of Lectures: 26
- Contact hours: ~4 hours/week
- Enrollment: 27-47

MENG 211 Thermodynamics for Mechanical Engineers, Yale University, Spring 2020, Fall 2020
- Course director

- Number of Lectures: 25
- Contact hours: ~4 hours/week
- Enrollment: 7-29

Physics 240A: Quantum Theory of Solids, UC Berkeley, Fall 2016

- Role: Graduate Student Instructor

Advising/Mentoring

Current Postdoctoral Advisees

- Dr. Victor Chang Lee, Yale University, 2022-present

Current Ph.D. Advisees

- Srikrishnaa Vadivel, Electrical Engineering, Yale University, 2022-Present
- Jinyuan Wu, MEMS, Yale University, 2022-present
- Xian Xu, Applied Physics, Yale University, 2022-present
- Bowen Hou, MEMS, Yale University, 2021-present
- (co-advisee) Luna Liu, Applied Physics, Yale University 2024-present
- (co-advisee) Alyssa Xu, MEMS, Yale University, 2023-present

Visiting Students

- Jiaxuan Guo, Fudan University, summer 2023

High School Students

- Henry Ding, Choate Rosemary Hall, summer 2023

Former Postdoctoral Advisees

- Dr. Aakash Kumar, Yale University, 2020-2022 -- Research scientist at Stony Brook University
- Dr. Dan Wang, Yale University, 2020-2022 – Assistant Professor at Beijing Institute of Technology

Former Ph.D. Advisees

- Chuanqi Xu, MEMS, Yale University, 2020 – joined Prof. Jakub Szefer's group in EECS at Yale
- Nicholas Richardson, MEMS, Yale University, 2022 – took leave of absence due to personal reasons
- Maria Belota Moreno, Physics, Yale University, 2023 – rotation student

Former Master's Advisees

- Aofeng (Barry) Bai, Applied Physics, Yale University, 2022

Former Undergraduate Research Advisees

- William (Jack) McArthur, Yale College, 2020-2022 – Ph.D. at UC Berkeley
- Tracy Lu, Tufts University, 2022
- Neal Ma, Yale College, 2021-2022
- Aditi Shetty, Yale College, 2021
- Charlie Loitman, Yale College, 2020

Other Teaching and Advising Contributions

Ph.D. Thesis Committee Member/Examiner

- Shunran Li, Yale University, 2020-present
- Salena Huang, Yale University, 2020-present

Ph.D. Thesis Reader

- Dr. Bradley Magnetta, Yale University, 2021
- Dr. Nicholas Lin Quan Cheng, National University of Singapore, 2021

Senior Essays Supervised

- Aditi Shetty, Yale College, 2021
- William (Jack) McArthur, Yale College 2022

Other Yale Service

Search Committees

- MEMS/ESI Search, 2022-present
  - Role: committee member
- MEMS Quantum Materials Search, 2021-2022
  - Role: Search Committee Chair
  - Hired: Cong Su
- CEE Search, 2021-2022
  - Role: committee member
  - No hire made

Other committee activity

- PSEB Phase II Committee, 2021-present
  - Role: committee member
  - Contributed to discussion about PSEB
- Materials Science exploratory committee, 2022-present
  - Role: committee member
  - Researched, discussed, and contributed to writing white paper on materials science at Yale
- MEMS Seminar committee, 2021-present
  - Role: main point of contact
  - Responsible for organizing and inviting MEMS seminar speakers
- MEMS Graduate Admission Committee, 2020-2022
  - Committee chair, 2020-2021
  - Committee member, 2022
  - Responsible for reviewing graduate applications and organizing graduate school open house

Outreach Activities at Yale

- Yale Graduate Women in Engineering and Applied Science Mentoring Group, 2023-present
  - Faculty mentor for a group of 5 women Ph.D. students in SEAS
- Yale IEEE Coffee chats with undergraduates, 2021
- Yale Science and Technology Research Scholar (STARS), 2020-present
  - Participated in Faculty Student Summer Research Matchmaking session, 2020
  - Volunteered to review undergraduate research proposals, 2020-present
- Yale Pathways Summer Scholars Workshop, Yale University, 2021
  - Organized and taught a 4-day computational materials science workshop for New Haven public high school students as part of the Yale Pathways to Science Summer Scholars Workshop. Students learned a general introduction to materials science and parallel computing and had the opportunity to run short simulations on Yale's High Performance Computing cluster.
- Yale Pathways to Science Summer Internship, 2022 – hosted Tracy Lu, Tufts University

Other Professional Service and Outreach

Grant Reviewer

- Department of Energy
- National Science Foundation
- European Research Council
- Deutsche Forschungsgemeinschaft (German Research Foundation)
- US-Israel Binational Science Foundation

Journal Referee

- *2D Materials, Advanced Materials, Applied Physics Letters, Journal of Chemical Physics, Materials Science in Semiconductor Processing, Nature, Nature Communications, Nature Physics, Nano Letters, NPJ Computational Materials, Physical Review B, Physical Review Letters, Physical Review Materials, Physical*

Review Research, Physics Communications, Proceedings of the National Academy of Sciences, Proceedings of the Royal Society A

Other Reviewing Activity

- National Academies draft report, "Frontiers in Synthetic Moiré Quantum Matter: Proceedings of a Workshop", 2021
- NSF Panels, 2021-2022

Developer of the open source BerkeleyGW code

- Core developer for the BerkeleyGW v2.0 release in 2018 and v3.0 release in 2021 -- Implemented non-uniform k-point sampling schemes, finite-momentum BSE (which allows for the calculation of exciton bandstructures), and bug-fixes for two-photon absorption processes
- BerkeleyGW performs *ab initio* calculations of single-particle and neutral excitations using the GW and GW plus Bethe Salpeter equation (GW-BSE) methods.

Non-Yale Mentoring and Outreach Activities

- Society of Women in the Physical Sciences, UC Berkeley, 2011-2016
- Berkeley Compass Project, UC Berkeley, 2013-2015
    - The Compass Project is a graduate student led group focused on improving science education and undergraduate student retention, especially from historically underrepresented groups and first-generation college students. Qiu participated in and led a small peer-mentoring group of graduate and undergraduate students.

Conferences and Workshops Organized

- BerkeleyGW Workshop and Conference, Co-Organizer, Berkeley, 2019-2022
- BerkeleyGW Workshop, Co-Organizer, Oakland, 2014-2018

Conference Sessions and Symposia Organized

- APS March Meeting, "Electronic Structure Methods for Excited States," Co-organizer, 2024
- APS March Meeting "APS March Meeting, "Electronic Structure Methods for Excited States," Co-organizer, 2024
- APS March Meeting, "Ultra-fast dynamics from electron-phonon interactions," Co-organizer, 2024
- MRS Spring Meeting, "Reconfiguring Properties of 2D Materials by Post-Synthesis Design," Co-Organizer, Honolulu, 2022
- APS March Meeting, "Probing Charge, Heat and Energy Transport at the Nanoscale," Co-Organizer, Chicago, 2022
- APS March Meeting, "Materials: Devices and Functionalities (DMP, DCOMP)," Co-Organizer, Chicago, 2022
- MRS Spring Meeting, "Excited State Properties of Materials—Theory and Computation," Co-Organizer, Virtual, 2021

Workshop Instructor

- BerkeleyGW Workshop and Conference, Berkeley, 2019-2022
- Electronic Structure Workshop, Merced, 2020
- BerkeleyGW Workshop, Oakland, 2014-2018

Other Service for Professional Organizations

- Department of Energy (DOE) Basic Energy Sciences (BES) Early Career Network (ECN) Representative, 2017-2020

Invited Talks

- **International Workshop on Computational Physics and Materials Science, "Progress in Electronic Structure Theory,"** Shanghai, China, 2024 (withdrew due to state department advisory)
- **International Conference on Functional Materials**, Kharagpur, India, 2024 (withdrew due to conflict)
- **13th International Conference on Excitonic and Photonic Processes in Condensed Matter and Nano Materials (Excon)**, Santa Fe, 2023

- **Sino-German Workshop: Optical Spectroscopy of 2D Semiconductors**, Xiamen, China, 2023 (withdrew due to state department advisory)
- **2D Transition Metal Dichalcogenides**, Cambridge, UK 2023
- **Oxford University,** Condensed Matter Seminar, Oxford, UK, 2023
- **Exciton Transport in 2D Materials**, San Sebastian, Spain, 2023
- **Los Alamos National Lab,** Condensed Matter Seminar, Los Alamos, 2023
- **Columbia University**, Quantum Materials Seminar, Virtual, 2023
- **MRS Spring Meeting**, San Francisco, 2023
- **Stony Brook University,** Condensed Matter Seminar, Stony Brook, 2023
- **NIST Quantum Matters in Materials Science Workshop**, Virtual, 2023
- **University of Washington in St. Louis**, Condensed Matter Seminar, St. Louis, 2022
- **MRS Fall Meeting**, Boston, 2022 (withdrew due to illness)
- **Packard Fellows Meeting**, Monterey, 2022
- **Psi-k Conference**, Lausanne, 2022
- **Gordon Research Conference,** Solid State Studies in Ceramics, Holyoke, 2022
- **Optica Advanced Photonics Congress**, Maastricht, 2022
- **MRS Spring Meeting**, Honolulu, 2022
- **Case Western Reserve University**, Condensed Matter Seminar, Virtual, 2022
- **CECAM Workshop on Exciton Dynamics in Functional Materials**, Virtual, 2021
- **Cambridge University**, Electronic Structure Seminar, Virtual, 2021
- **Temple University,** Physics Colloquium, Virtual, 2021
- **MRS/Kavli Future of Materials Workshop**, Virtual, 2021
- **MRS Spring Meeting**, Virtual, 2021
- **APS March Meeting**, Virtual, 2021
- **University of Washington Seattle,** Materials Colloquium, Virtual, 2021
- **CECAM Workshop on GW-XL**, Virtual, 2020
- **Yale University**, Physics Colloquium, New Haven, 2020
- **Weizmann Institute of Science**, Materials Science Seminar, Rehovet, 2019
- **Cambridge University,** Condensed Matter Seminar, Cambridge, 2019
- **University of Regensburg**, Condensed Matter Seminar, Regensburg, 2019
- **Fudan University**, Condensed Matter Seminar, Shanghai, 2019
- **Shanghai Jiao Tong University,** Condensed Matter Seminar, Shanghai, 2019
- **Notre Dame University,** Physics Colloquium, South Bend, 2019
- **Yale University,** Materials Science Seminar, New Haven, 2019
- **Ohio State University,** Physics Colloquium, Columbus, 2019
- **Stanford University,** Materials Science Seminar, Palo Alto, 2019
- **Hebrew University of Jerusalem,** Physics Colloquium, Jerusalem, 2019
- **University of Pennsylvania,** Physics Colloquium, Philadelphia, 2019
- **University of California Berkeley**, Pitzer Seminar in Theoretical Chemistry, Berkeley, 2019
- **BerkeleyGW Workshop and Conference**, Oakland, 2019
- **APS March Meeting,** New Orleans, 2017
- **27th Annual Workshop on Recent Developments in Electronic Structure Theory**, Seattle, 2015

Contributed Presentations at Conferences and Workshops

- **APS March Meeting**, Las Vegas, 2023
- **APS March Meeting**, Chicago, 2022
- **APS March Meeting**, Boston, 2019
- **APS March Meeting**, New Orleans, 2017

- **ECRC-HUB-CMS PI Meeting**, Washington D.C., 2017
- **APS March Meeting**, Baltimore, 2016
- **APS March Meeting**, San Antonio, 2015
- **APS March Meeting**, Denver, 2014
- **APS March Meeting**, Baltimore, 2013