

Diana Y. Qiu

Assistant Professor

Department of Mechanical Engineering and Materials Science
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Employment

Assistant Professor, 2020-present, Yale University, New Haven, CT, USA

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

DOE Early Career Award, 2021

Co-PI on DOE INCITE Award, 2019 (renewed in 2020)

Project title: “*Novel Methods for Complex Excited-State Phenomena in Functional Materials*”

The Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program allocates large amounts of resources at the US Department of Energy (DOE) Leadership Computing Facilities for “transformational advances in science and technology.”

Rising Stars in Physics Workshop, Massachusetts Institute of Technology, 2018

One of ~25 invited attendees at a workshop aimed at bringing “the next generation of physics academic leaders together for two days of scientific discussions and informal sessions aimed at navigating the early stages of the academic career”

EFRC-Hubs-CMS PI Meeting Team Science Competition, 2017

Graduate student and postdoc presentation award at the biennial PI meeting of DOE Energy Frontier Research Centers (EFRC), Hubs, and Computational Materials Science (CMS) centers

Jackson C. Koo Award, 2017

Awarded annually to a senior graduate student in condensed matter physics at UC Berkeley

National Science Foundation Graduate Research Fellowship, 2011-2016

Berkeley Chancellor’s Fellowship, 2011-2013

Howard L. Schultz Prize, 2011

Barry Goldwater Scholarship, 2010

Publications in Journals

(Publication Highlights: Published 31 articles, cited 4,000+ times, h-index=18)

*=corresponding author (last author unless otherwise noted)

†=equal contribution

1. 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," in press *Nature Communications*, arXiv:2006.14705 (2020).
2. 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).
 3. E. Mitterreiter, B. Schuler, A. Micevic, D. Hernangómez-Pérez, K. Barthelmi, K.A. Cochran, 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).
 4. 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)
 5. 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.
 6. H.M. Bretscher, Z. Li, J. Xiao, **D.Y. Qiu**, S. Refaely-Abramson, J. Alexander-Webber, A.O.A. Tanoh, Y. Fan, G. Delpont, 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).
 7. S. Yazdani, J.V. Pondick, A. Kumaar, M. Yarali, J.M. Woods, D.J. Hynes, **D.Y. Qiu**, J.J. Cha, "Heterointerface effects on lithium-induced phase transitions in intercalated MoS₂," *ACS Applied Material Interfaces*, 13 10603-10611 (2021).
 8. 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).
 9. **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**.
 10. **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).
 11. 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).
 12. 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 WS₂," *Physical Review Letters* 123, 07681 (2019).
Chosen as **Editor's Suggestion**.
 13. 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).
 14. 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).
 15. 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)
 16. 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 MoS₂," *J. Phys. Chem. C*, 121, 22559-22566 (2017).
 17. **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).
 18. 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).

19. 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 MoS₂," *Physical Review B*, 95, 115407 (2017).
20. 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).
21. 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).
22. **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie, "Screening and many-body effects in two-dimensional crystals: Monolayer MoS₂," *Physical Review B*, 93, 235435 (2016).
23. 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 BaTiO₃/(2×1)-Ge(001) Interface," *Physical Review Letters*, 116, 106101 (2016).
24. **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**.
25. 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 MoSe₂ Nanostructures," *Nano Letters*, 15, 2594-2599 (2015).
26. 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).
27. 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).
28. 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).
29. **D. Y. Qiu**, F. H. da Jornada, and S. G. Louie, "Optical spectrum of MoS₂: many-body effects and diversity of exciton states," *Physical Review Letters*, 111, 216805 (2013). Erratum: *Phys Rev Lett*, 115, 119901 (2015).
30. **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).
31. 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

1. **D.Y. Qiu***, G. Cohen, D. Novichkova, S. Refaely-Abramson*, "Novel Signatures of Dimensionality and Symmetry in Exciton Bandstructure: Consequences for Time-Evolution," *submitted*, arXiv:2103.07514 (2021).
2. 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," *submitted*, arXiv: arXiv:2107.09635 (2021).
3. 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 heterostructures," *submitted*, arXiv:2107.02255 (2021).
4. C. Zhang, F. Tang, M. Chen, 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," *submitted*, arXiv:2104.14410 (2021).

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).

Grants & Funding

"First Principles Approach to Exciton Transport in Energy Materials"

D. Y. Qiu (PI), \$750,000, 2021-2026

DOE Early Career Research Program

"Ab Initio Downfolding Approach to Dynamical Exciton-Continuum Interactions"

D. Y. Qiu (PI), \$363,725, 2021-2024

NSF Condensed Matter and Materials Theory Program

"Center for the Computational Study of Excited State Phenomena in Energy Materials (C2SEPEM)"

S. G. Louie (PI), \$600,000 (Yale sub-award), 2020-2024

DOE Computational Materials Science Center

Invited Talks

2021

MRS/Kavli Future of Materials Virtual Workshop

Invited Talk: "Towards Ab Initio Theory of Exciton Transport and Diffusion"

MRS Spring Meeting Virtual

Invited Talk: "Subspace Embedding and Downfolding Techniques for Solving the Bethe Salpeter Equation"

APS March Meeting Virtual

Invited Talk: "Subspace Embedding and Downfolding Techniques for Solving the Bethe Salpeter Equation: Interplay of Localized and Continuum Excitons in Complex Systems"

Materials Colloquium University of Washington, Seattle

2020

GW-XL Helsinki, Finland

Invited Talk: "Scaling up Ab-Initio MBPT Calculations for Nanostructured Systems: Applications to Defects and Core-Level Excitations"

Physics Colloquium Yale University

2019

Materials Seminar Weizmann Institute of Science

Condensed Matter Seminar Cambridge University

Condensed Matter Seminar University of Regensburg

Condensed Matter Seminar Fudan University

Condensed Matter Seminar Shanghai Jiao Tong University

Physics Colloquium Notre Dame University

Materials Science Seminar Yale University

Physics Colloquium Ohio State University

Physics Colloquium Boston College

Materials Science Seminar Stanford University

Physics Colloquium Hebrew University of Jerusalem

Condensed Matter Seminar University of Pennsylvania

Pitzer Seminar in Theoretical Chemistry UC Berkeley

BerkeleyGW Workshop and Conference, Oakland, CA

Invited Talk: "Solving the BSE for Systems of Mixed Localization: Implications for Defects and Singlet-Triplet Splitting"

2017

APS March Meeting, New Orleans, LA

Invited Talk: “Many-Body Effects on the Electronic and Optical Properties of Quasi-2D Semiconductors”

2015

27th Annual Workshop on Recent Developments in Electronic Structure Theory, Seattle, WA

Invited Talk: “Many-body effects on the electronic and optical properties of quasi two-dimensional materials”

Teaching

MENG 280 Strength and Deformation of Materials, Yale University, Fall 2021

MENG 492/ENAS 755 Electronic and Optical Properties of Energy Materials, Yale University, Spring 2021

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

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

As Graduate Student Instructor

Mentoring

Postdoctoral Advisees

Dr. Aakash Kumar (2020-present)

Dr. Dan Wang (2020-present)

Graduate Research Advisees

Chuanqi Xu (2020)

Undergraduate Research Advisees

Aditi Shetty (2021)

Jack McArthur (2020-present)

Charlie Loitman (2020)

Professional Service and Outreach

Grant Reviewer

Department of Energy, National Science Foundation, European Research Council

Referee

2D Materials, Advanced Materials, Applied Physics Letters, Journal of Chemical Physics, Materials Science in Semiconductor Processing, Nature, Nature Communications, Nano Letters, NPJ Computational Materials, Physical Review B, Physical Review Letters, Physical Review Materials, Physical Review Research, Physics Communications, Proceedings of the Royal Society A

Developer of the open source BerkeleyGW code

BerkeleyGW performs *ab initio* calculations of single-particle and neutral excitations using the GW and GW plus Bethe Salpeter equation (GW-BSE) methods.

Core developer for the BerkeleyGW v2.0 release in 2018 and v3.0 release in 2021 -- Implemented non-uniform k-point sampling schemes, bug-fixes for two-photon absorption processes, and finite-momentum BSE, which allows for the calculation of exciton bandstructures

Mentoring and Outreach Activities

Yale Science and Technology Research Scholar (STARS) 2020-present Yale University

The STARS program is designed to support women, minority, economically underprivileged, and other historically underrepresented students in the sciences, engineering, and mathematics.

Participated in Faculty Student Summer Research Matchmaking session.

Volunteered to review undergraduate research proposals.

Society of Women in the Physical Sciences 2011-2016 UC Berkeley

Participated in and led small peer mentoring groups.

Berkeley Compass Project 2013-2015 UC Berkeley

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.

Participated in and led a small peer-mentoring group of graduate and undergraduate students.

Conferences and Workshops Organized

BerkeleyGW Workshop and Conference	Co-Organizer	2021	Berkeley, CA
Steven G. Louie 70 th Birthday Symposium	Co-Organizer	2019	Berkeley, CA
BerkeleyGW Workshop and Conference	Co-Organizer	2019	Oakland, CA
BerkeleyGW Workshop	Co-Organizer	2018	Oakland, CA
BerkeleyGW Workshop	Co-Organizer	2017	Oakland, CA
BerkeleyGW Workshop	Co-Organizer	2016	Oakland, CA
BerkeleyGW Workshop	Co-Organizer	2015	Oakland, CA
BerkeleyGW Workshop	Co-Organizer	2014	Oakland, CA

Conference Sessions and Symposia Organized

MRS Spring Meeting	Co-Organizer	2021	Virtual Meeting
Symposium Title: "Excited State Properties of Materials—Theory and Computation"			

Conference Sessions Chaired

APS March Meeting	2021	Virtual Meeting
APS March Meeting	2017	New Orleans, LA

Workshop Instructor

BerkeleyGW Workshop and Conference	2021	Berkeley, CA
Electronic Structure Workshop	2020	Merced, CA
BerkeleyGW Workshop and Conference	2019	Oakland, CA
BerkeleyGW Workshop	2018	Oakland, CA
BerkeleyGW Workshop	2017	Oakland, CA
BerkeleyGW Workshop	2016	Oakland, CA
BerkeleyGW Workshop	2015	Oakland, CA
BerkeleyGW Workshop	2014	Oakland, CA

Service for Professional Organizations

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

Organized and invited speakers for panels on energy science career-paths, grant writing and diversity.

Contributed Presentations at Conferences and Workshops

2019

APS March Meeting, Boston, MA

2018

APS March Meeting, Los Angeles, CA

2017

APS March Meeting, New Orleans, LA

ECRC-HUB-CMS PI Meeting, Washington D.C.

2016

APS March Meeting, Baltimore, MD

2015

APS March Meeting, San Antonio, TX

2014

APS March Meeting, Denver, CO

2013

APS March Meeting, Baltimore, MD