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Research Interests

- Materials for electronic and optoelectronic devices
- Density functional theory and electronic structure methods

Current Research Topics

- Electric polarization, piezoelectricity, and flexoelectricity
- Functional properties of semiconductors and complex oxides
- Electron-phonon coupling
- Point defects in semiconductors and insulators
- Quantum embedding methods for correlated materials

Education

2015 Postdoctoral Associate, Physics, Rutgers University; Advisor: David Vanderbilt
2014 Postdoctoral Researcher, Materials, UC Santa Barbara; Van de Walle Group
2014 Ph.D. in Materials, UC Santa Barbara; Advisor: Chris G. Van de Walle
2009 B.S. High Honors, in Engineering Science, Physics, and Mathematics (minor in Materials Science), University of Virginia

Publications

1. Gabriel I. López-Morales, Joanna M. Zajac, Tom Delord, Carlos A. Meriles, Cyrus E. Dreyer, "Density-functional theory study of the interaction between NV centers and native defects in diamond," *arXiv:2507.22683*
2. Jennifer Coulter, Fabian B. Kugler, Harrison LaBollita, Antoine Georges, Cyrus E. Dreyer "Mechanisms for the ultralow room-temperature resistivity of $SrMoO_3$," *arXiv:2506.10143*
3. Guadalupe García-Arellano, Gabriel I López Morales, Zav Shotan, Raman Kumar, Ben Murdin, Cyrus E Dreyer, Carlos A Meriles, "Erbium-Implanted WS2 Flakes with Room-Temperature Photon Emission at Telecom Wavelengths," Nano Letters **25** (22), 9070-9076 (2025).
4. Harrison LaBollita, Jeremy Lee-Hand, Fabian B Kugler, Lorenzo Van Muñoz, Sophie Beck, Alexander Hampel, Jason Kaye, Antoine Georges, Cyrus E Dreyer, "Low-temperature transport in high-conductivity correlated metals: a density-functional plus dynamical mean-field study of cubic perovskites," *arXiv:2505.04508*
5. Kevin G. Kleiner, Sonali Joshi, Woncheol Lee, Alexander Hampel, Malte Rösner, Cyrus E. Dreyer, Lucas K. Wagner"Quantum Monte Carlo assessment of embedding for a strongly-correlated defect: interplay between mean-field and interactions," *arXiv:2505.00845.*
6. Harikrishnan KP, Varun Harbola, Jaehong Choi, Kevin J. Crust, Yu-Tsun Shao, Chia-Hao Lee, Dasol Yoon, Yonghun Lee, Gregory D Fuchs, Cyrus E. Dreyer, Harold Y.

Hwang, David A. Muller, “Microscopic mechanisms of flexoelectricity in oxide membranes,” *arXiv:2503.12984*

7. Asier Zabalo, Cyrus E. Dreyer, Massimiliano Stengel, “Static Born charges and quantum capacitance in metals and doped semiconductors,” *Phys. Rev. B* **111**, 094307 (2025), *arXiv:2501.10303.*
8. Sakal Singla, Pragya Joshi, Gabriel I López-Morales, Kenji Watanabe, Takashi Taniguchi, Cyrus E Dreyer, Biswanath Chakraborty, “Direct Observation of Optically Active Mid-Gap Electronic States in Hexagonal Boron Nitride by Electron Spectroscopy,”*Advanced Materials*, 2502342 (2025).
9. Jeremy Lee-Hand, Harrison LaBollita, Fabian B. Kugler, Lorenzo Van Muñoz, Jason Kaye, Sophie Beck, Alexander Hampel, Antoine Georges, Cyrus E. Dreyer, “Fermi-Liquid T^2 Resistivity: Dynamical Mean-Field Theory Meets Experiment,” *arXiv:2412.16363*
10. Gabriel I. López-Morales, Joanna M. Zajac, Johannes Flick, Carlos A. Meriles, Cyrus E. Dreyer, “Quantum embedding study of strain- and electric-field-induced Stark effects on the NV^- center in diamond,” *Phys. Rev. B* **110**, 245127 (2024), *arXiv:2406.07772*
11. Xie Zhang, Mark E Turiansky, Lukas Razinkovas, Marek Maciaszek, Peter Broqvist, Qimin Yan, John L. Lyons, Cyrus E. Dreyer, Darshana Wickramaratne, Ádám Gali, Alfredo Pasquarello, and Chris G. Van de Walle, “First-principles calculations of defects and electron–phonon interactions: Seminal contributions of Audrius Alkauskas to the understanding of recombination processes,” *J. Appl. Phys.* **135**, 150901 (2024).
12. Yueqing Chang, Erik G. C. P. van Loon, Brandon Eskridge, Brian Busemeyer, Miguel A. Morales, Cyrus E. Dreyer, Andrew J. Millis, Shiwei Zhang, Tim O. Wehling, Lucas K. Wagner, Malte Rösner, “Downfolding from Ab Initio to Interacting Model Hamiltonians: Comprehensive Analysis and Benchmarking,” *npj Comput.l Mater.* **10**, 129 (2024), *arXiv:2311.05987*
13. Shang Ren, John Bonini, Massimiliano Stengel, Cyrus E. Dreyer, David Vanderbilt, “Adiabatic dynamics of coupled spins and phonons in magnetic insulators,” *Phys. Rev. X* **14**, 011041 (2024), *arXiv:2307.05668*
14. Cyrus E. Dreyer, Rouven Essig, Marivi Fernandez-Serra, Aman Singal, Cheng Zhen, “Fully ab-initio all-electron calculation of dark matter–electron scattering in crystals with evaluation of systematic uncertainties,” *Phys. Rev. D* **109**, 115008 (2024), *arXiv:2306.14944*
15. Danis I. Badrtdinov, Carlos Rodriguez-Fernandez, Magdalena Grzeszczyk, Zhizhan Qiu, Kristina Vaklinova, Pengru Huang, Alexander Hampel, Kenji Watanabe, Takashi Taniguchi, Lu Jiong, Marek Potemski, Cyrus E. Dreyer, im, Malte Rösner, “Dielectric environment sensitivity of carbon centres in hexagonal boron nitride,” *Small*, 2300144 (2023), *arXiv:2305.08240*
16. Santiago Perez, Dario Rodrigues, Juan Estrada, Roni Harnik, Zhen Liu, Brenda A. Cervantes-Vergara, Juan Carlos Dolivo, Ryan D. Plestid, Javier Tiffenberg, Tien-Tien Yu, Alexis Aguilar-Arevalo, Fabricio Alcalde-Bessia, Nicolas Avalos, Oscar Baez, Daniel Baxter, Xavier Bertou, Carla Bonifazi, Ana Botti, Gustavo Cancelo, Nuria Castello-Mor, Alvaro E. Chavarria, Claudio R. Chavez, Fernando Chierchie, Juan Manuel De Egea, Cyrus Dreyer, Alex Drlica-Wagner, Rouven Essig, Ezequiel Estrada, Erez Etzion, Paul Grylls, Guillermo Fernandez-Moroni, Marivi Fernandez-Serra, Santiago Ferreyra, Stephen Holland, Agustin Lantero Barreda, Andrew Lathrop, Ian Lawson, Ben Loer, Steffon Luoma, Edgar Marrufo Villalpando, Mauricio Martinez Montero, Kellie McGuire, Jorge Molina, Sravan Munagavalasa, Danielle Norcini, Alexander Piers, Paolo Privitera, Nathan Saffold, Richard Saldanha, Aman Singal, Radomir Smida, Miguel Sofo-Haro, Diego Stalder, Leandro Stefanazzi, Michelangelo

Traina, Yu-Dai Tsai, Sho Uemura, Pedro Ventura, Rocio Vilar Cortabitarte, Rachana Yajur, "Early Science with the Oscura Integration Test," *arXiv:2304.08625*

17. Brenda A. Cervantes-Vergara, Santiago Perez, Juan Estrada, Ana Botti, Claudio R. Chavez, Fernando Chierchie, Nathan Saffold, Alexis Aguilar-Arevalo, Fabricio Alcalde-Bessia, Nicolás Avalos, Oscar Baez, Daniel Baxter, Xavier Bertou, Carla Bonifazi, Gustavo Cancelo, Nuria Castelló-Mor, Alvaro E. Chavarria, Juan Manuel De Egea, Juan Carlos D'Olivo, Cyrus Dreyer, Alex Drlica-Wagner, Rouven Essig, Ezequiel Estrada, Erez Etzion, Paul Grylls, Guillermo Fernandez-Moroni, Marivi Fernández-Serra, Santiago Ferreyra, Stephen Holland, Agustín Lantero Barreda, Andrew Lathrop, Ian Lawson, Ben Loer, Steffon Luoma, Edgar Marrufo Villalpando, Mauricio Martinez Montero, Kellie McGuire, Jorge Molina, Sravan Munagavalasa, Danielle Norcini, Alexander Piers, Paolo Privitera, Dario Rodrigues, Richard Saldanha, Aman Singal, Radomir Smida, Miguel Sofo-Haro, Diego Stalder, Leandro Stefanazzi, Michelangelo Traina, Sho Uemura, Pedro Ventura, Rocío Vilar Cortabitarte, Rachana Yajur, "Skipper-CCD Sensors for the Oscura Experiment: Requirements and Preliminary Tests," *arXiv:2304.04401*
18. John Bonini, Shang Ren, David Vanderbilt, Massimiliano Stengel, Cyrus E. Dreyer, Sinisa Coh, "Frequency splitting of chiral phonons from broken time reversal symmetry in CrI3," *Phys. Rev. Lett.* **130**, 086701 (2023), *arXiv:2208.14593*
19. Sara Shabani, Thomas P. Darlington, Colin Gordon, Wenjing Wu, Emanuil Yanev, James Hone, Xiaoyang Zhu, Cyrus E. Dreyer, P. James Schuck, Abhay N. Pasupathy, "Ultra Localized Optoelectronic Properties of Nanobubbles in 2D Semiconductors," *Nano Lett.* **18**, 7401 (2022), *arXiv:2208.14518*.
20. E. Cappelli, A. Hampel, A. Chikina, E. Bonini Guedes, G. Gatti, A. Hunter, J. Issing, N. Biskup, M. Varela, Cyrus E. Dreyer, A. Tamai, A. Georges, F.Y. Bruno, M. Radovic, F. Baumberger, "Electronic structure of the highly conductive perovskite oxide SrMoO3," *Phys. Rev. Materials* **6**, 075002 (2022). *arXiv:*2203.05820
21. Alexis Aguilar-Arevalo, Fabricio Alcalde Bessia, Nicolas Avalos, Daniel Baxter, Xavier Bertou, Carla Bonifazi, Ana Botti, Mariano Cababie, Gustavo Cancelo, Brenda Aurea Cervantes-Vergara, Nuria Castello-Mor, Alvaro Chavarria, Claudio R. Chavez, Fernando Chierchie, Juan Manuel De Egea, Juan Carlos D`Olivo, Cyrus E. Dreyer, Alex Drlica-Wagner, Rouven Essig, Juan Estrada, Ezequiel Estrada, Erez Etzion, Guillermo Fernandez-Moroni, Marivi Fernandez-Serra, Steve Holland, Agustin Lantero Barreda, Andrew Lathrop, Jose Lipovetzky, Ben Loer, Edgar Marrufo Villalpando, Jorge Molina, Santiago Perez, Paolo Privitera, Dario Rodrigues, Richard Saldanha, Diego Santa Cruz, Aman Singal, Nathan Saffold, Leandro Stefanazzi, Miguel Sofo-Haro, Javier Tiffenberg, Christian Torres, Sho Uemura, Rocio Vilar, "The Oscura Experiment," *arXiv*:2202.10518.
22. Vidushi Sharma, Benjamin Bein, Amanda Lai, Betül Pamuk, Cyrus E. Dreyer, Marivi Fernández-Serra, Matthew Dawber, "Cooperative Interactions between Surface Terminations Explain Photocatalytic Water Splitting Activity on SrTiO3," *Phys. Rev. X Energy* **1**, 023002 (2022), *arXiv:2201.13443*
23. Asier Zabalo, Cyrus E. Dreyer, Massimiliano Stengel, "Rotational *g* factors and Lorentz forces of molecules and solids from density-functional perturbation theory," *Phys. Rev. B* **105**, 094305 (2022). *arXiv*:2112.11946.
24. Lukas Muechler, Danis I. Badrtdinov, Alexander Hampel, Jennifer Cano, Malte Rösner, Cyrus E. Dreyer, "Quantum embedding methods for correlated excited states of point defects: Case studies and challenges," *Phys. Rev. B* **105**, 235104 (2022), *arXiv*:2105.08705.

25. Danis I. Badrtdinov, Alexander Hampel, Cyrus E. Dreyer, "Interplay between breathing-mode distortions and magnetic order in rare-earth nickelates from ab initio magnetic models," *Phys. Rev. B* **104**, 054403 (2021), *arXiv*:2103.08412.
26. Cyrus E. Dreyer, Sinisa Coh, Massimiliano Stengel, "Nonadiabatic Born effective charges in metals and the Drude weight," *Phys. Rev. Lett.* **128**, 095901 (2022). **Editor's Suggestion.** *arXiv*:2103.044251.
27. Alexander Hampel, Jeremy Lee-Hand, Antoine Georges, Cyrus E. Dreyer, "Correlation-Induced Octahedral Rotations in SrMoO3," *Phys. Rev. B* **104**, 035102 (2021) *arXiv*:2012.07871
28. Nicholas L. Adamski, Cyrus E. Dreyer, and Chris G. Van de Walle, "Polarization properties at rocksalt/wurtzite oxide interfaces," *Phys. Rev. B* **102**, 201301(R) (2020)
29. Mark E. Turiansky, Audrius Alkauskas, Manuel Engel, Georg Kresse, Darshana Wickramaratne, Jimmy-Xuan Shen, Cyrus E. Dreyer, Chris G. Van de Walle "Nonrad: Computing Nonradiative Capture Coefficients from First Principles," *Comput. Phys Commun.* **267**, 108056 (2021), *arXiv*:2011.07433
30. Jeremy Lee-Hand, Alexander Hampel, Cyrus E. Dreyer "First-principles study of the electronic, magnetic, and crystal structure of perovskite molybdates," *Phys. Rev. Materials* **5**, 085001 (2021). *arXiv*:2011.08323
31. Cyrus E. Dreyer, Audrius Alkauskas, John L. Lyons, and Chris G. Van de Walle, "Radiative capture rates at deep defects from electronic structure calculations," *Phys. Rev. B* **102**, 085305 (2020), *arXiv*:2008.02732
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33. Aldo H. Romero, Douglas C. Allan, Bernard Amadon Gabriel Antonius, Thomas Applencourt, Lucas Baguet, Jordan Bieder, François Bottin, Johann Bouchet, Eric Bousquet, Fabien Bruneval, Guillaume Brunin, Damien Caliste, Michel Côté, Jules Denier, Cyrus Dreyer, Philippe Ghosez, Matteo Giantomassi, Yannick Gillet, Olivier Gingras, Donald R. Hamann, Geoffroy Hautier, François Jollet, Gérald Jomard, Alexandre Martin, Henrique P. C. Miranda, Francesco Naccarato, Guido Petretto, Nicholas A. Pike, Valentin Planes, Sergei Prokhorenko, Tonatiuh Rangel, Fabio Ricci, Gian-Marco Rignanese, Miquel Royo, Massimiliano Stengel, Marc Torrent, Michiel J. van Setten, Benoit Van Troeye, Matthieu J. Verstraete, Julia Wiktor, Josef W. Zwanziger, and Xavier Gonze, "ABINIT: Overview and focus on selected capabilities," *J. Chem. Phys.* **152**, 124102 (2020).
34. Vatsal A. Jhalani, Jin-Jian Zhou, Jinsoo Park, Cyrus E. Dreyer, Marco Bernardi, "Piezoelectric Electron-Phonon Interaction from Ab Initio Dynamical Quadrupoles: Impact on Charge Transport in Wurtzite GaN," *Phys. Rev. Lett.* 125, 136602 (2020), *arXiv*:2002.08351
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36. L. J. McGilly, A. Kerelsky, N. R. Finney, K. Shapovalov, E.-M. Shih, A. Ghiotto, Y. Zeng, S. L. Moore, W. Wu, Y.Bai, K. Watanabe, T. Taniguchi, M. Stengel, L. Zhou, J. Hone, X.-Y. Zhu, D.N. Basov, C. Dean, C. E. Dreyer, and A. N. Pasupathy, "Visualization of moiré superlattices," *Nature Nanotechnology* 15, 580 (2020), *arXiv*:1912.06629
37. Darshana Wickramaratne, Cyrus E. Dreyer, Jimmy-Xuan Shen, John L. Lyons, Audrius Alkauskas, and Chris G. Van de Walle, "Deep-Level Defects and Impurities in InGaN Alloys," *Phys. Status Solidi B.* **257**,1900534 (2019). **Featured Article.**

38. Nicholas L. Adamski, Cyrus E. Dreyer, Chris G. Van de Walle, "Giant polarization charge density at lattice-matched GaN/ScN interfaces" *Appl. Phys. Lett.* **115**, 232103 (2019). *arXiv*:1910.00142
39. Darshana Wickramaratne, Jimmy-Xuan Shen, Cyrus E. Dreyer, Audrius Alkauskas, and Chris G. Van de Walle, "Electrical and optical properties of iron in GaN, AlN, and InN," *Phys. Rev. B* **99**, 205202 (2019).
40. Andrea Schiaffino, Cyrus E. Dreyer, David Vanderbilt, and Massimiliano Stengel, "Metric-wave approach to flexoelectricity within density-functional perturbation theory," *Phys. Rev. B* **99**, 085107 (2019). **Editor's Suggestion.** *arXiv*:1811.12893
41. Darshana Wickramaratne, Cyrus E. Dreyer, Bartomeu Monserrat, Jimmy-Xuan Shen, John L. Lyons, Audrius Alkauskas, Chris G. Van de Walle, "Defect identification based on first-principles calculations for deep level transient spectroscopy," *Appl. Phys. Lett.* **113**, 192106 (2018). **Featured Article**. *arXiv:*1810.05302
42. Cyrus E. Dreyer, Massimiliano Stengel, David Vanderbilt, "Current-density implementation for calculating flexoelectric coefficients," *Phys. Rev. B* **98**, 075153 (2018). **Editor's Suggestion.** *arXiv*:1802.06390
43. Cyrus E. Dreyer, Audrius Alkauskas, John L. Lyons, Anderson Janotti, and Chris G. Van de Walle, "First-principles calculations of point defects for quantum technologies," *Annu. Rev. Mater. Res.,* **48**, 2.1 (2018).
44. Bartomeu Monserrat, Cyrus E. Dreyer, Karin M. Rabe, "Phonon-assisted optical absorption in BaSnO3 from first principles," *Phys. Rev. B* **97**, 104310 (2018). *arXiv*:1709.09196
45. Richard C. Cramer, Bastien Bonef, John English, Cyrus E. Dreyer, Chris G. Van de Walle, and James S. Speck, "Growth of coherent BGaN films using BBr3 gas as a boron source in plasma assisted molecular beam epitaxy," *J. Vac. Sci. Technol. A* **35**, 041509 (2017). **Editor's pick**.
46. Jimmy-Xuan Shen, Darshana Wickramaratne, Cyrus E. Dreyer, Audrius Alkauskas, Erin Young, James S. Speck, and Chris G. Van de Walle, "Calcium as a nonradiative recombination center in InGaN," *Appl. Phys. Express*, **10**, 021001 (2017).
47. Darshana Wickramaratne, Jimmy-Xuan Shen, Cyrus E. Dreyer, Manuel Engel, Martijn Marsman, Georg Kresse, Saulius Marcinkevicius, Audrius Alkauskas, and Chris G. Van de Walle, "Iron as a source of efficient Shockley-Read-Hall recombination in GaN," *Appl. Phys. Lett.,* **109**, 162107 (2016).
48. Kevin R. Bagnall, Cyrus E. Dreyer, David Vanderbilt, and Evelyn N. Wang, "Electric Field Dependence of Optical Phonon Frequencies in Wurtzite GaN Observed in GaN High Electron Mobility Transistors," *J. Appl. Phys.* **120**, 155104 (2016).
49. Hiral D. Tailor, John L. Lyons, Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "Impact of nitrogen and carbon on defect equilibrium in ZrO_2," *Acta Materialia,* **117**, 286 (2016).
50. Cyrus E. Dreyer, Anderson Janotti, Chris G. Van de Walle, and David Vanderbilt, "Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides," *Phys. Rev. X,* **6**, 021038 (2016). *arXiv*:1605.07629
51. Audrius Alkauskas, Cyrus E. Dreyer, John L. Lyons, and Chris G. Van de Walle, "Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors," *Phys. Rev. B* **93**, 201304(R) (2016). **Editor's Suggestion.** *arXiv*:1605.05673
52. Cyrus E. Dreyer, Audrius Alkauskas, John L. Lyons, James S. Speck, and Chris G. Van de Walle, "Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters," *Appl. Phys. Lett.* **108**, 141101 (2016). **Selected for feature article and issue cover.**

53. Patrick M. McBride, Anderson Janotti, Cyrus E. Dreyer, Burak Himmetoglu, and Chris G. Van de Walle, "Effects of biaxial stress and layer thickness on octahedral tilts in LaNiO3," *Appl. Phys. Lett.* **107**, 261901 (2015).
54. Karthik Krishnaswamy, Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "First-principles study of surface charging in $LaAlO_3/SrTiO_3$ heterostructures," *Phys. Rev. B* **92**, 085420 (2015).
55. Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "Brittle fracture toughnesses of GaN and AlN from first-principles surface-energy calculations." *Appl. Phys. Lett.* **106**, 212103 (2015).
56. Karthik Krishnaswamy, Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "Structure and energetics of $LaAlO_3$ (001) surfaces," *Phys. Rev. B* **90**, 235436 (2014).
57. Cyrus E. Dreyer, John L. Lyons, Anderson Janotti, and Chris G. Van de Walle, "Band alignments and polarization properties of BN polymorphs," *Appl. Phys. Express* **7**, 031001 (2014).
58. Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "Absolute surface energies of polar and nonpolar planes of wurtzite GaN," *Phys. Rev. B* **89**, 081305(R) (2014). **Editor's Suggestion.**
59. Cyrus E. Dreyer, Anderson Janotti, and Chris G. Van de Walle, "Effects of strain on the electron effective mass in GaN and AlN," *Appl. Phys. Lett.* **102**, 142105 (2013).
60. Cyrus E. Dreyer, William V. Chiu, Robert H. Wagoner, and Sean R. Agnew, "Formability of a More Randomly Textured Magnesium Alloy Sheet: Application of an Improved Warm Sheet Formability Test," *J. Mater. Process Tech.* **210**, 37 (2010).

Reference Module

1. "Point Defects and Impurities in III-Nitride Bulk and Thin Film Heterostructures", C. E. Dreyer and C. G. Van de Walle, in *Reference Module in Materials Science and Materials Engineering*, edited by S. Hashmi (Elsevier, Oxford, 2016), pp. 1-8.

Invited Talks/Seminars

1. "Fermi-Liquid T^2 Resistivity: Dynamical Mean-Field Theory Meets Experiment," DMFT-QE Symposium (virtual), September 2025
2. "Beyond Born-Oppenheimer in metals and magnets," Physics department colloquium, SUNY Binghampton, Binghampton, NY, September 2025
3. "Fermi-Liquid T^2 Resistivity: Dynamical Mean-Field Theory Meets Experiment," Berkeley Excited States Conference, Berkeley, CA, August 2025
4. "Effective models and quantum embedding for defects," Materials Research Society spring meeting, Seattle, WA, April 2025
5. "Excited states of strongly correlated point defects using quantum embedding methods," APS March Meeting, Anahaim, CA, March 2025
6. "NV center quantum metrology for radiation damage in materials," Materials Research Society fall meeting, Boston, MA, December 2024
7. "Quantum embedding for point defects: Case studies and challenges," Electronic Devices Seminar, Cornell, May 2024
8. "Quantum embedding for point defects," CECAM Defects in solids for quantum technologies, Budapest, Hungary, June 2024
9. "Benchmarking quantum embedding for point defects: The case of Fe in AlN," International Conference on Advanced Materials and Devices, Jeju, Korea, December 2023
10. "First-principles methods for phonons in magnetic systems," CCQ-CIFAR Quatum Materials workshop, Flatiron CCQ, New York, NY, November 2023

11. “Nonadiabatic lattice dynamics in metals and magnets,” Condensed Matter Group seminar, University of Connecticut, Storrs, CT, October, 2023
12. “Beyond Born-Oppenheimer in metals and magnets,” Physics department colloquium, CCNY, New York, NY, October, 2023
13. “Nonadiabatic lattice dynamics in metals and magnets,” Seminar, University of Helsinki, Finland, September 2023
14. “Phonons from density functional theory,” African School on Electronic Structure methods and applications, June 2023, Kigali, Rwanda
15. “Quantum embedding methods for point defects: Case studies and challenges,” Quantum Foundry seminar, Santa Barbara, CA, May 2023
16. “Quantum embedding methods for point defects: Case studies and challenges,” ACS Spring meeting, Indianapolis, IN, March 2023
17. “Interplay between structure, magnetism, and correlations in molybdate and nickelate perovskite oxides,” Seminar at Purdue University, West Lafayette, IN, March 2023
18. “Nonadiabatic lattice dynamics in metals and magnets,” 21st International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, Trieste, Italy, January 2023
19. “Quantum embedding methods for point defects: Case studies and challenges,” GRC on Defects in Semiconductors, New London, NH, August 2022
20. “Interplay between structure, magnetism, and correlations in molybdate and nickelate perovskite oxides,” Seminar at Institut de Ciència de Materials de Barcelona, Barcelona, Spain, July 2022
21. “Computational spectroscopy for point defects,” APS March Meeting, Chicago, Il, March 2022
22. “The method of long waves: New *ab initio* results from a classic technique,” Seminar, UIUC Institute for Condensed Matter Theory, Champaign, IL (virtual), October 2021
23. “Computational spectroscopy for point defects,” International Conference on Defects in Semiconductors (Plenary talk), Oslo, Norway (virtual), July 2021
24. “Understanding solids with supercomputers, many electrons at a time,” Aspen Center for Physics public lecture, Aspen, Co, July 2021
25. “Nonadiabatic Born effective charges in metals and the Drude weight,” Ferrolectures series (virtual), June 2021
26. “First-principles calculations of point defects for quantum applications,” Flatiron Institute CCQ Seminar, New York, NY (virtual), May 2020
27. “Flexoelectricity in 2D materials,” Stony Brook Condensed Matter Seminar, Stony Brook NY (virtual), May 2020
28. “Understanding solids with supercomputers, many electrons at a time,” Stony Brook World of Physics, Stony Brook NY, February 2020
29. “Electron-phonon coupling from first principles: Novel implementations and applications,” BNL CFN Seminar, Upton NY, December 2019
30. “Theoretical identification and characterization of point defects,” CUNY physics department colloquium, New York, NY, October 2019
31. “The modern theory of polarization with a twist,” Lehigh physics department colloquium, Bethlehem, PA, September 2019
32. “Performing and interpreting first-principles calculations for point-defect properties,” International Conference on Defects in Semiconductors, Seattle, WA, July 2019
33. “Flexoelectricity from first principles,” Theory of Condensed Matter Seminar, Radboud University, Nijmegen, The Netherlands, May 2019
34. “Flexoelectricity from first principles,” Theory of Condensed Matter seminar, Cambridge University, Cambridge, UK, May 2019

35. “Current-density implementation for calculating flexoelectric coefficients of cubic oxides,” Electronic Materials and Applications 2019, Orlando, FL, January 2019
36. “Flexoelectricity from first principles,” Materials department seminar, Santa Barbara, CA, January 2019
37. “Electron-phonon coupling from first principles: Novel implementations and applications,” MRSEC Seminar, Columbia University, New York, NY, January 2019
38. “Current-density implementation for calculating flexoelectric coefficients,” Electronic Structure Workshop, Philadelphia, PA, June 2018
39. “Current-density implementation for calculating flexoelectric coefficients,” Materials Science and Technology Division seminar, United States Naval Research Laboratory, Washington D.C., June 2018
40. "Carrier capture and recombination at point defects from first principles,” APS User Meeting, Argonne National Lab, Agonne, IL, May 2018
41. “Electron-phonon coupling from first principles: Novel implementations and applications,” Department of Physics and Astronomy seminar, Stony Brook University, Stony Brook, NY, February 2018
42. “Electron-phonon coupling from first principles: Novel implementations and applications,” Flatiron Institute Center for Computational Quantum Physics, New York, NY, February 2018
43. “Sources of Shockley-Read-Hall in III-nitrides,” International Conference on Defects in Semiconductors, Matsue, Japan, August 2017
44. “The role of electron-phonon coupling in carrier capture at defects,” APS March Meeting, New Orleans, LA, March 2017
45. “Shockley-Read-Hall recombination from first principles: Improving the efficiency of III-nitride devices,” Institut de Ciència de Materials de Barcelona seminar, Barcelona, Spain, July 2016
46. “Sources of Shockley-Read-Hall recombination in III-Nitrides,” Condensed Matter Seminar, UC Santa Cruz, Santa Cruz, CA, October 2016
47. "Radiative capture of carriers at defects from first principles," Northrup-Grumman Next Workshop on Physics of Light-matter Interactions and Excited State Dynamics, Redondo Beach, CA, October, 2016
48. “Sources of Shockley-Read-Hall recombination in III-Nitrides,” Institute for Energy Efficiency seminar, UC Santa Barbara, Santa Barbara, CA, October, 2016
49. “Sources of Shockley-Read-Hall recombination in III-Nitrides,” Center for Computational Design of Functional Layered Materials seminar, Temple University, Philadelphia, PA, October, 2016
50. “Accurate treatment of spontaneous polarization in III-nitrides,” International Symposium of Semiconductor Light Emitting Devices, Kaohsiung, Taiwan, December, 2014
51. “Spontaneous polarization in III-nitrides and the importance of a consistent reference structure,” Nitrides Seminar, UC Santa Barbara, Santa Barbara, CA, May 2014
52. “Absolute surface energies of polar and non-polar planes in GaN,” Nitrides Seminar, UC Santa Barbara, Santa Barbara, CA, November, 2012

Contributed talks

1. “Benchmarking quantum embedding for point defects: The case of Fe in AlN,” International conference on defects in semiconductors, Rehoboth Beach, Delaware, September 2023
2. “Long-wavelength expansion of electrical polarization: Recent results from a classic method,” Fundamental physics of ferroelectrics and related materials, Golden, CO, February 2023

3. “First-principles calculations of flexoelectricity in bulk boron nitride,” Fundamental physics of ferroelectrics and related materials, Silver Spring, MD, January 2020
4. “Current density at finite q for clamped-ion flexoelectricity,” Abinit developers meeting, Louvain-la-Neuve, Belgium, May 2019
5. “Current-density implementation for calculating flexoelectric coefficients,” APS March Meeting, Los Angeles, CA, March 2018
6. “Current-density implementation for calculating flexoelectric coefficients,” 32nd Annual Symposium of the Laboratory for Surface Modification and Institute for Advanced Materials, Devices, and Nanotechnology, Piscataway, NJ, February 2018
7. “Current-density implementation for calculating flexoelectric coefficients,” Fundamental Physics of Ferroelectrics, Washington D.C., January 2018
8. “Current-density implementation for calculating flexoelectric coefficients,” APS Mid-Atlantic Section Meeting, Newark, NJ, November 2017
9. “Correct implementation of polarization constants in wurtzite materials and impact on III-nitrides,”APS March Meeting, New Orleans, LA, March 2017
10. “Sources of Shockley-Read-Hall recombination in III-nitride light emitters,” APS March Meeting, Baltimore, MD, March 2016
11. “Accurate treatment of spontaneous polarization in III-nitrides,” APS March Meeting, San Antonio, TX, March 2015
12. “Absolute surface energies, fracture toughness, and cracking in nitrides,” International Workshop on Nitrides, Wroclaw, Poland, August, 2014
13. “Absolute surface energies, fracture toughness, and cracking in nitrides,” APS March Meeting, Denver, CO, March 2014
14. “Absolute surface energies, fracture toughness, and cracking in nitrides,” Solid State Lighting and Energy Center Review, Santa Barbara, CA, November 2013
15. “Absolute surface energies of polar and nonpolar planes in GaN,” International Conference on Nitride Semiconductors, Washington D.C., August, 2013
16. “Absolute surface energies of polar and nonpolar planes in GaN,” APS March Meeting, Baltimore, MD, March, 2013
17. “Absolute surface energies of polar and non-polar planes in GaN,” Annual Meeting of the California-Nevada Section of the APS, San Luis Obispo, CA, November, 2012
18. “Surface energies and cracking in GaN,” APS March Meeeting, Boston, MA, March, 2012
19. “Effects of strain on effective masses in GaN and AlN,” TMS Electronic Materials Conference, Santa Barbara, CA, June 2011
20. “Effects of strain on effective masses in GaN and AlN,” APS March Meeting, Dallas, TX, March, 2011
21. “Extracting post-uniform constitutive behavior from high temperature tensile test data,” TMS Annual Meeting, Seattle, WA, February, 2010

Awards

2022 NSF CAREER award

2017 Poster Award for: “Towards a supercell-free current-based calculation of flexoelectric couplings,” presented at Fundamental Physics of Ferroelectrics, 2017

2013 Finalist in Grad Slam three-minute research talk competition

2013 Solid State Lighting and Energy Center Outstanding Graduate Student Research Achievement Award

Press Coverage

1. “LED Lighting May Now Shine Brighter: Scientists apprehended the atomic-scale, microscopic mechanism that limits light emission in LED lighting,” News Wise, March 1, 2017
2. “LEDs: Resolving the iron conundrum,” Compound Semiconductor, December 2016
3. “Trace amounts of transition-metal impurities in GaN kill LED efficiency,” Semiconductor Today, November 11, 2016
4. “Trace metal recombination centres kill LED efficiency,” Compound Semiconductor, November 7, 2016
5. “Trace metal recombination centers kill LED efficiency,” AAAS Eureka Alert, November 3, 2016
6. “Supercomputers Help Identify Efficiency-Limiting Defects in LEDs,” NERSC.gov, July 18, 2016
7. “Correcting charge polarization calculations for III-nitrides,” Semiconductor Today, July 6, 2016
8. “LED lighting may now shine brighter,” US DOE Office of Science, Science Highlight, July 1, 2016
9. “Unraveling the nature of point defects in nitride LEDs,” Compound Semiconductor, June 4, 2016
10. “Defects in LED diodes that lead to less efficient solid state lighting identified,” Energy Daily, April 13, 2016
11. “Certain type of vacancy in gallium nitride based LEDs lowers their efficiency,” Laser Focus World, April 11, 2016
12. “Identifying defects in LED materials promises more efficient lighting,” Smart2Zero, April 7, 2016
13. “Researchers identify specific defects in LED diodes that lead to less efficient solid state lighting,” Phys.org, Science Daily, AAAS Eureka Alert, April 6, 2016
14. “Becoming Crystal Clear: UCSB researchers identify specific defects in LED diodes that lead to less efficient solid state lighting,” The UC Santa Barbara Current, April 5, 2016
15. “Theoretical technique identifies defects in LED materials,” Photonics Media, April 2016
16. “Aiding nitride growth with accurate surface energies,” Compound Semiconductor, May 19, 2014

Professional Activities

2025:	Organized symposium for 2025 PsiK conference
2024-2025:	On the steering committee for International Conference on Nitride Semiconductors
2024-2025:	Organized invited symposia on Quantum Information Science for Materials Physics and Electronic Structure for Dark Matter detection for 2025 APS Global Physics Summit
2023-2025:	Organized focus session on recent applications and developments in quantum embedding at the 2023 APS March Meeting
2023:	Lectured at African School on Electronic Structure Methods and Applications
2023:	Panelist for Stony Brook Physics and Astronomy Undergraduate Research Day
2022:	Organized session on recent developments and applications of DFT+DMFT at the 33rd IUPAP Conference on Computational Physics
2021:	Co-organized the International Workshop on Recent Developments in Electronic Structure (ES21).
2020-2024:	Co-organized 2020, 2021, and 2024 Fundamental Physics of Ferroelectrics workshop

2019-present:	Reviewed proposals for National Science Foundation, Israeli Ministry of Innovation, Science and Technology, ACS Petroleum Research Fund
2019:	Taught python programming to high school students at “IACS Computes” programming camp
2019:	Organized Defects and Dopants in Semiconductors Focus Session at 2019 APS March Meeting
2017-2019:	Member of advisory committee for International Conference on Defects in Semiconductors
2018:	Chair of 2018 Gordon Research Seminar on Defects in Semiconductors
2014:	Selected by the Dean of the Graduate Division to meet with local lawmakers at California Graduate Research Advocacy Day
2014:	Selected for Communications Committee of UCSB Institute for Energy Efficiency
2011-2021:	Reviewed manuscripts for: Physical Review Applied, Physical Review B, Physical Review Letters, Physical Review Materials, Physical Review Applied, Applied Physics Letters, Nano Letters, Journal of Electronic Materials, Journal of Applied Physics, Physica Status Solidi B, Journal of Crystal Growth, New Journal of Chemistry, RSC Advances, Advanced Materials Interfaces, Surface Science Reports, Nanophotonics