Qimin Yan

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Education

2007-2012 **Ph. D in Materials**, Materials Department, University of California, Santa Barbara
Supervisor: Prof. Chris G. Van de Walle and Prof. Matthias Scheffler
Thesis: Theoretical Study of Material and Device Properties of Group-III Nitrides

2003-2006 **M. S. in Physics**, Department of Physics, Tsinghua University, China

1999-2003 **B. S. in Applied Physics**, Dept. of Applied Physics, Xi'an Jiaotong University, China

Professional Experience

2016- present Assistant Professor,
Department of Physics, Temple University

2013-2016 Post-doctoral researcher,
Molecular Foundry, Lawrence Berkeley National Laboratory
Department of Physics, University of California, Berkeley
Supervisor: Prof. Jeffrey B. Neaton

2012 Post-doctoral researcher,
Materials Department, University of California, Santa Barbara
Supervisor: Prof. Chris G. Van de Walle

Awards and Fellowships

2022 NSF CAREER Award, National Science Foundation

2021 Selected as "Emerging Leaders 2021" by Journal of Physics: Condensed Matter.

2020 Finalist for "2020 Rising Stars in Computational Materials Science Prize"

2019 DOE Early Career Award, Department of Energy

2017 NERSC Award for High Impact Scientific Achievement

2011 Outstanding Graduate Student Research Achievement Award,
Solid-State Lighting and Energy Center, University of California, Santa Barbara.

2006 Excellent Master's Thesis Award, Tsinghua University, China

Professional Activities

- Conference organization: Co-organizer for the Focus Topic "Computational Discovery and Design of Novel Materials" in APS March Meeting 2017; Co-organizer of the symposium "2D Layered Materials Beyond Graphene—Theory, Discovery and Design" in MRS Spring Meeting 2019
- Proposal Review: NSF OAX SSE; NSF Division of Materials Research; DOE BES Early Career Program; DOE Quantum Information Science Program; DOE EPSCoR Program; Proposal review board member for the Center for Nanoscale Materials at Argonne National Laboratory.
- Referee of Physical Review Letters, ACS Nano, Materials Today, Nano Letters, npj Computational Materials, Chemical Communications, Chemistry of Materials, Physical Chemistry Chemical Physics, Applied Physics Letters, Journal of Applied Physics, Journal of Physics: Condensed Matter, Journal of Materials Chemistry A, Computational Materials Science, Journal of Nanomaterials, etc.

- Member of American Physical Society and Materials Research Society.

Teaching Experience

Temple University

Fall 2021	Physics 1062 - Elementary Classical Physics II
Spring 2021	Physics 2511 - Scientific Computing I
	Physics 4511 - Scientific Computing III
Fall 2020	Physics 1062 - Elementary Classical Physics II
Spring 2020	Physics 4511 - Scientific Computing III
Fall 2019	Physics 8702 - Solid State Physics
Spring 2019	Physics 8702 - Solid State Physics
Fall 2018	Physics 2021 - General Physics
Spring 2018	Physics 8702 - Solid State Physics
Fall 2017	Physics 1061 - Elementary Classical Physics I
Fall 2016	Physics 1061 - Elementary Classical Physics I

Mentoring Experience

Temple University

2021-present	Anoj Aryal, Graduate Student
	Alex Heilman, Graduate Student
	Debajit Chakraborty, Research Assistant Professor
2020-present	Andy Philips, Undergraduate Student
2020-2021	Brendan Magdamo, Undergraduate Student
2019-present	Weiyi Gong, Graduate Student
2019-2020	Lifu Zhang, Visiting Student
2019 summer	Francesco Ricci, Visiting Scholar
2018-present	Jeng-Yuan Tsai, Graduate Student
2018-2020	Yijun Tong, Visiting Master Student
	(Now as a PhD student at University of Washington)
2017	Linh Nguyen, Undergraduate Student
2017	Dylan Harrison, Undergraduate Student
2016-2020	Huta R Banjade, Graduate Student
	(Now as a Postdoc Fellow at Virginia Commonwealth University)
	Yu Wang, Undergraduate Student
	(Now as a PhD student at Princeton University)
2016-2019	Jinbo Pan, Postdoc Fellow
	(Now as an Associate Professor at Chinese Academy of Sciences)
	Yanfang Zhang, Visiting Scholar
	(Now as a Postdoc Fellow at Chinese Academy of Sciences)

2016-2018 Liping Yu, Research Assistant Professor
(Now as an Assistant Professor at University of Maine)

Lawrence Berkeley National Laboratory & UC Berkeley

2015-2016 Sophie Weber, graduate student supervised by Jeffrey Neaton
2013-2014 Tess Smidt, graduate student supervised by Jeffrey Neaton
2014 Aditi Krishnapriyan, undergraduate student, SULI Summer intern
2013 Bryan A. Smith, undergraduate student, SULI Summer intern

Funding ($1.97 M since 2016)

2022–2027 National Science Foundation, Faculty Early Career Development Program (CAREER), $507,958, "CAREER: Quantum defects in two-dimensional materials by local-symmetry-guided data-driven design". (PI)

2019 – 2024 Department of Energy, Early Career Research Program, $750,000, "Synthesis of motif and symmetry for accelerated learning, discovery, and design of electronic structures for energy conversion applications". (PI)

2018 – 2022 Department of Energy, Quantum Information Science Program, $405,226, "Design, Control and Application of Next-Generation Qubits". (PI at Temple)

2018 – 2020 Department of Energy, EFRC Center, $110,582, "Center for Complex Materials from First Principles (CCM)". (co-PI)

2016 – 2018 Department of Energy, EFRC Center, $200,000, "Center for the Computational Design of Functional Layered Materials (CCDM)". (co-PI)

Invited Presentations

1. Condensed Matter Seminar, Stony Brook University, NY (2021)
   Data-driven materials design in the quantum regime
2. Department of Materials Science and Engineering, University of Pennsylvania, PA (2021)
   Data-driven materials design in the quantum regime
3. Physics Colloquium, Temple University, Philadelphia, PA (2020)
   Symmetry enabled effective learning and accelerated discovery of quantum materials
4. SCAN Workshop, Temple University, Philadelphia, PA (2019)
   Data-driven discovery of functional 2D materials using a SCAN-enabled electronic structure database
5. Department of Physics, Penn State University, University Park, PA (2018)
   Data-driven discovery of functional 2D materials utilizing a 2D electronic structure database
6. Lecture Series on Materials Theory and Computation, Xi'an, China (2018)
   Data-driven discovery of functional 2D materials
7. Department of Applied Physics & Materials, California Institute of Technology, CA (2018)
   Data-driven discovery of functional 2D materials utilizing a 2D electronic structure database

8. International Conference on Low-dimensional Quantum Materials, Snowbird, UT (2018)

   Data-driven discovery of functional 2D materials utilizing a 2D electronic structure database

9. MSE Colloquium, Boston University, MA (2017)

   Discovery of functional energy and topological materials with a combination of high-throughput theory and experiment

10. College of Materials Science & Engineering, Jilin University, Changchun, China (2017)

    Data-driven discovery of solar fuels photoanode materials

11. Institute of Physics, Chinese Academy of Science, China (2017)

    Discovery of solar fuels photoanode materials with a combination of high-throughput theory and experiment

12. Department of Physics, Xi'an Jiaotong University, Xi'an, China (2017)

    Discovery of solar fuels photoanode materials with a combination of high-throughput theory and experiment

13. Hefei National Laboratory for Physical Sciences at the Microscale, USTC, Hefei, China (2017)
    Discovery of solar fuels photoanode materials with a combination of high-throughput theory and experiment
14. Beijing Computational Science Research Center, Beijing, China (2017)
    Materials Genome Initiative and data-driven discovery of solar fuels photoanode materials
15. Electronic Materials and Applications 2017, Orlando, FL (2017)

    Discovery of solar fuels photoanode materials by integrating high-throughput theory and experiment

16. Department of Materials Science and Engineering, University of Michigan, Ann Arbor, MI (2016)
    First-principles data-driven discovery of transition metal oxides for artificial photosynthesis
17. Department of Materials Engineering, Purdue University, West Lafayette, IN (2016)

    Predictive design of functional materials and devices: from high-throughput computation to multi-scale modeling

18. Department of Materials Science and Engineering, University of California, Riverside, CA (2016)

    Discovery and design of functional materials and devices: from high-throughput calculations to multi-scale modeling

19. American Physical Society March Meeting 2016, Baltimore, MD (2016)

    First-principles data-driven discovery of transition metal oxides for artificial photosynthesis

20. Department of Physics & Astronomy, Rutgers University, Piscataway, NJ (2016)

    Discovery and design of complex materials with ab initio high-throughput approaches

21. Department of Materials Science and Engineering, University of Delaware, DE (2015)

    Computational design of new materials for energy applications: from high-throughput calculations to multi-scale modeling

22. Department of Physics, Xi'an Jiaotong University, China (2015)

Materials genome initiative and data-driven discovery of novel energy and topological materials

23. Department of Materials Science and Engineering, Shanghai Jiaotong University, China (2015)
    Materials genome initiative and data-driven discovery of novel energy and topological materials
24. Materials Genome Institute, Shanghai University, China (2015)

    Materials genome initiative and data-driven discovery of novel energy and topological materials

25. School of Physics, Nankai University, China (2015)

    Materials genome initiative and data-driven discovery of novel energy and topological materials

26. Institute of Physics, Chinese Academy of Science, China (2015)

    Materials genome initiative and data-driven discovery of novel energy and topological materials

27. Division of Energy & Environment, Shenzhen Graduate School of Tsinghua University, China (2015)

    Materials genome initiative and data-driven discovery of novel energy and topological materials

28. Department of Materials Science and Engineering, Tsinghua University, China (2015)

    Materials genome initiative and data-driven discovery of novel energy and topological materials

29. Materials Department, University of California, Santa Barbara, CA (2014)

    Ab Initio high-throughput approach for discovery of stable transition metal oxides for solar energy capture and conversion

30. Molecular Foundry, Lawrence Berkeley National Laboratory, CA (2012)

    Theoretical Study of Material and Device Properties of Group-III Nitrides

31. Department of Physics, Tsinghua University, China (2011)

    The role of nitrogen vacancies and related complexes in the luminescence and p-type doping compensation of GaN

32. Nano Science Center of Copenhagen University, Copenhagen University, Denmark (2006)

    Electronic structure and transport property of carbon ribbons

Publications

72 scientific publications; **1** U.S. patent; **1** book chapter.

Google Scholar link: https://scholar.google.com/citations?user=ysfTfdkAAAAJ&hl=en

Total citations: **4792**; h-index: **34**; **16** publications with over 100 citations.

72 J.-Y. Tsai, J. Pan, H. Lin, A. Bansil, **Q. Yan**, "Antisite defect qubits in monolayer transition metal dichalcogenides", ***Nat. Commun.*** 13, 492 (2022)

71 J.-Y. Tsai, **Q. Yan**, "Perspective: Spin-Dependent Phenomena in Two-Dimensional Materials"**.** ***Phys. Chem. Chem. Phys.*** *accepted* (2022)

70 H. Bai, P. Chu, J. Y. Tsai, N. Wilson, X. Qian, **Q. Yan**, H. Ling, "Graph Neural Network for Hamiltonian-Based Material Property Prediction" ***Neural. Comput. Applic.*** (2021)

69 M. Richter, E. Peterson, L. Zhou, A. Shinde, P. Newhouse, **Q. Yan**, S. Fackler, J. Yano, J. Cooper, K. Persson, J. Neaton, J. Gregoire, "Band Edge Energy Tuning Through Electronic Character Hybridization in Ternary Metal Vanadates" ***Chem. Mater.*** 33, 7242 (2021)

68 H. R. Banjade, S. Hauri, S. Zhang, F. Ricci, W. Gong, G. Hautier, S. Vucetic, **Q. Yan**, "Structure motif centric learning framework for inorganic crystalline systems", ***Sci. Adv.***, 7, eabf1754 (2021)

67 W. Gong, **Q. Yan**, "Graph-based deep learning frameworks for molecules and solid-state materials", ***Comput. Mater. Sci.*** 195, 110332 (2021)

66 Y. F. Zhang, J. Pan, H. Banjade, J. Yu, H. Lin, A. Bansil, S. Du, **Q. Yan**, "Two-dimensional MX Dirac materials and quantum spin Hall insulators with tunable electronic and topological properties", ***Nano Res.*** 14, 584 (2021)
Selected as cover article

65 H. R. Banjade, J. Pan, **Q. Yan,** "Monolayer 2D semiconducting tellurides for high-mobility electronics" ***Phys. Rev. Mater.*** 5, 014005 (2021)

64 N. H. Attanayake, H. R. Banjade, A. C. Thenuwara, B. Anasori, **Q. Yan**, D. R. Strongin, "Electrocatalytic CO_2 reduction on Earth Abundant 2D Mo_2C and Ti_3C_2 MXenes", ***Chem. Commun.*** 57, 1675 (2021)

63 F. Hu, S. C. Abeyweera, J. Yu, D. Zhang, Y. Wang, **Q. Yan**, Y. Sun, "Quantifying Electrocatalytic Reduction of CO_2 on Twin Boundaries" ***Chem*** 6, 3007 (2020)

62 L. Zhang, J. Pan, **Q. Yan**, Z. Hu, "Computational Study of the Novel 2D Ferromagnetic Metal: Ce_2C Monolayer", ***Phys. Status Solidi RRL***, 14, 2000324 (2020)

61 J. Pan, Y. F. Zhang, J. Zhang, H. Banjade, J. Yu, L. Yu, S. Du, A. Ruzsinszky, Z. Hu, **Q. Yan**, "Auxetic two-dimensional transition metal selenides and halides" ***npj Comput. Mater.*** 6, 154 (2020)

60 J. Pan, J. B. Yu, Y. F. Zhang, S. Du, A. Janotti, C. X. Liu, **Q. Yan**, "Quantum anomalous Hall effect in two-dimensional magnetic insulator heterojunctions" ***npj Comput. Mater.*** 6, 152 (2020)

59 S. C. Abeyweera, J. Yu, J. P. Perdew, **Q. Yan**, Y. Sun, "Hierarchically 3D Porous Ag Nanostructures Derived from Silver Benzenethiolate Nanoboxes: Enabling CO2 Reduction with a Near-Unity Selectivity and Mass-Specific Current Density over 500 A/g" ***Nano Lett.*** 20, 2806 (2020)

58 C. Li, N. Ku, Y. Liu, J. Pan, B. Chai, F. Hu, M. Kornecki, **Q. Yan**, R. Brennan, S. Ren, "Magnetically active transition metal cation-substituted alumina" ***Nanotechnology*** 31, 105703 (2019)

57 L. Yu, A. Ruzsinszky, **Q. Yan,** "Chemisorption Can Reverse Defect–Defect Interaction on Heterogeneous Catalyst Surfaces" ***J. Phys. Chem. Lett.*** 10, 7311 (2019)

56 L. Yu, **Q. Yan**, and A. Ruzsinszky, "Key role of antibonding electron transfer in bonding on solid surfaces", ***Phys. Rev. Materials*** 3, 092801 (2019)

55 J. Zeng, Y. F. Zhang, W. Qin, P. Cui, **Q. Yan**, Z. Zhang, "Varying topological properties of two-dimensional honeycomb lattices composed of endohedral fullerenes" **Phys. Rev. B** 100, 045143 (2019)

54 N. K. Nepal, L. Yu, **Q. Yan**, and A. Ruzsinszky, "First-principles study of mechanical and electronic properties of bent monolayer transition metal dichalcogenides", ***Phys. Rev. Mater.*** 3, 073601 (2019)

53 W. Zhang, Y. Hu, J. Pan, J. Zhang, J. Cui, **Q. Yan**, S. Ren, "High current carrying and thermal conductive copper-carbon conductors.", ***Nanotechnology***, 30, 185701 (2019)

52 Y. Sun, J. Pan, Z. Zhang, K. Zhang, J. Liang, W. Wang, Z. Yuan, Y. Hao, Y. Hao, B. Wang, J. Wang, Y. Wu, J. Zheng, L. Jiao, S. Zhou, K. Liu, C. Cheng, W. Duan, Y. Xu, **Q. Yan**, K. Liu, "Elastic Properties and Fracture Behaviors of Biaxially-Deformed, Polymorphic $MoTe_2$", ***Nano Lett.***, 19, 761 (2019)

51 A. C. Thenuwara, L. Dheer, N. H. Attanayake, **Q. Yan**, U. V. Waghmare, D. R. Strongin, "Co-Mo-P Based Electrocatalyst for Superior Reactivity in the Alkaline Hydrogen Evolution Reaction", ***Chem. Cat. Chem.*** 10, 4832 (2018)

50 Q. Zhou, P. Tang, S. Liu, J. Pan, **Q. Yan**, S. -C. Zhang, "Learning atoms for materials discovery", ***PNAS*** 115, E6411 (2018)

49 J. Pan, **Q. Yan**, "Data-driven material discovery for photocatalysis: a short review",

48 D. Lee, H. Wang, B. A. Noesges, T. J. Asel, J. Pan, J.-W. Lee, **Q. Yan**, L. J. Brillson, X. Wu, C.-B. Eom, "Identification of a functional point defect in $SrTiO_3$", ***Phys. Rev. Mat.*** 2, 060403 (2018)

47 A. Thenuwara, N. Attanayake, J. Yu, J. Perdew, E. Elzinga, **Q. Yan**, D. Strongin, "Cobalt Intercalated Layered NiFe Double Hydroxides for the Oxygen Evolution Reaction", ***J. Phys. Chem. B*** 122, 847 (2018)

46 S. K. Suram, L. Zhou, A. Shinde, **Q. Yan**, J. Yu, M. Umehara, H. S. Stein, J. B. Neaton, J. M. Gregoire, "Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes", ***Chem. Commun.*** 54, 4625 (2018)

45 S. F. Weber, R. Chen, **Q. Yan**, J. B. Neaton, "Prediction of TiRhAs as a Dirac nodal line semimetal via first-principles calculations", ***Phys. Rev. B*** 96, 235145 (2017)

44 J. Wang, X. Sui, W. Shi, J. Pan, S. Zhang, F. Liu, S.-H. Wei, **Q. Yan**, B. Huang, "Prediction of Ideal Topological Semimetals with Triply Degenerate Points in the $NaCu_3Te_2$ Family", ***Phys. Rev. Lett.*** 119, 256402 (2017)

43 A. Shinde, S. Suram, **Q. Yan**, L. Zhou, A. Singh, J. Yu, K. Persson, J. B. Neaton, J. Gregoire, "Discovery of manganese-based solar fuels photoanodes via integration of electronic structure

calculations, Pourbaix stability modeling, and high throughput experiments", ***ACS Energy Lett.*** 2, 2307 (2017)

42 C. Jones, C. H. Teng, **Q. Yan**, P. C. Ku, E. Kioupakis, "Impact of carrier localization on recombination in InGaN quantum wells and the efficiency of nitride light-emitting diodes: Insights from theory and numerical simulations", ***Appl. Phys. Lett.*** 111, 113501 (2017)

41 **Q. Yan**, J. Yu, S. K. Suram, L. Zhou, A. Shinde, P. Newhouse, W. Chen, G. Li, K. A. Persson, J. M. Gregoire, J. B. Neaton, "Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment", ***PNAS*** 114, 3040 (2017)
Selected as DOE Science Highlight and awarded the NERSC Award for High Impact Scientific Achievement.

40 C. F. Wu, H. Wang, **Q. Yan**, T. R. Wei, J. F. Li, "Doping of thermoelectric PbSe with chemically inert secondary phase nanoparticles" ***J. Mater. Chem. C*** 5, 10881 (2017)

39 Y. S. Guan, Z. Zhang, J. Pan, **Q. Yan**, S. Ren, "Rational design of molecular crystals for enhanced charge transfer properties", ***J. Mater. Chem. C*** 5, 12338 (2017)

38 L. Yu, **Q. Yan**, A. Ruzsinszky, "Negative Poisson's Ratio in 1T-Type Crystalline Two-Dimensional Transition Metal Dichalcogenides", ***Nat. Commun.*** 8, 15224 (2017)

37 C. Freysoldt, B. Lange, J. Neugebauer, **Q. Yan**, J. L. Lyons, A. Janotti, C. G. Van de Walle, "Electron and chemical reservoir corrections for point-defect formation energies", ***Phys. Rev. B*** 93, 165206 (2016)

36 A. Shinde, G. Li, L. Zhou, D. Guevarra, S. K. Suram, F. M. Toma, **Q. Yan**, J. A. Haber, J. B. Neaton, J. M. Gregoire, "The role of the CeO2/BiVO4 interface in optimized Fe–Ce oxide coatings for solar fuels photoanodes", ***J. Mater. Chem. A*** 4, 14356 (2016)

35 L. Zhou, **Q. Yan**, J. Yu, R. J. Jones, N. Becerra-Stasiewicz, S. K. Suram, A. Shinde, D. Guevarra, J. B. Neaton, K. A Persson, J. M. Gregoire, "Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation", ***Phys. Chem. Chem. Phys.*** 18, 9349 (2016)

34 L. Zhou, **Q. Yan**, A. Shinde, D. Guevarra, P. F. Newhouse, N. Becerra-Stasiewicz, S. M. Chatman, J. A Haber, J. B. Neaton, J. M. Gregoire, "High Throughput Discovery of Solar Fuels Photoanodes in the CuO–V_2O_5 System", ***Adv. Energy Mater.*** 5, 1500968 (2015)
Highlighted by the Joint Center for Artificial Photosynthesis.

33 C. Pan, **Q. Yan**, H. Fu, Y. Zhao, Y. Wu, C. G. Van de Walle, S. Nakamura, S. P. DenBaars, "High optical power and low-efficiency droop blue light-emitting diodes using compositionally step-graded InGaN barrier", ***Electronics Lett.*** 51, 1187 (2015)

32 **Q. Yan**, G. Li, P. F. Newhouse, J. Yu, K. Persson, J. M. Gregoire, J. B. Neaton, "$Mn_2V_2O_7$: An Earth Abundant Light Absorber for Solar Water Splitting", ***Adv. Energy Mater.*** 5, 1401840 (2015)
Highlighted by the Joint Center for Artificial Photosynthesis.

31 J. Yu, **Q. Yan**, W. Chen, A. Jain, J. B. Neaton and K. Persson, "First-principles study of electronic structure and photocatalytic properties of $MnNiO_3$ as an alkaline oxygen-evolution photocatalyst", ***Chem. Commun.*** 51, 2867 (2015)

30 **Q. Yan**, A. Janotti, M. Scheffler, Chris G. Van de Walle, "Origins of optical absorption and emission lines in AlN", ***Appl. Phys. Lett.*** 105, 111104 (2014)

29 **Q. Yan**, P. Rinke, A. Janotti, M. Scheffler, C. G. Van de Walle, "Effects of strain on the band structure of wurtzite group-III nitrides", ***Phys. Rev. B*** 90, 125118 (2014)

28 **Q. Yan**, E. Kioupakis, D. Jena, and C. G. Van de Walle, "First-principles study of high-field related electronic behavior of group-III nitrides", ***Phys. Rev. B*** 90, 121201(R) (2014)

27 P. M. McBride, **Q. Yan**, and C. G. Van de Walle, "Effects of In profile on simulations of InGaN/GaN multi-quantum-well light-emitting diodes", ***Appl. Phys. Lett.*** 105, 083507 (2014)

26 A. Alkauskas, **Q. Yan**, C. G. Van de Walle, "First-principles theory of nonradiative carrier capture via multiphonon emission", ***Phys. Rev. B*** 90, 075202 (2014)
Selected as "Editor's suggestions" on Phys. Rev. B.

25 K. Liu, **Q. Yan**, M. Chen, W. Fan, Y. Sun, J. Suh, D. Fu, S. Lee, J. Zhou, S. Tongay, J. Ji, J. B. Neaton, J. Wu, "Elastic Properties of Chemical-Vapor-Deposited Monolayer MoS_2, WS_2, and Their Bilayer Heterostructures", ***Nano Lett.*** 14, 5097 (2014)

24 N. Wang, D. West, J. Liu, J. Li, **Q. Yan**, B. L. Gu, S. B. Zhang, W. H. Duan, "Microscopic origin of the p-type conductivity of the topological crystalline insulator SnTe and the effect of Pb alloying", ***Phys. Rev. B*** 89, 045142 (2014)

23 E. Kioupakis, **Q. Yan**, and C. G. Van de Walle, "Temperature and carrier-density dependence of Auger and radiative recombination in nitride optoelectronic devices", ***New J. Phys.*** 15, 125006 (2013)

22 M. S. Miao, **Q. Yan**, C. G. Van de Walle, "Electronic structure of a single-layer InN quantum well in a GaN matrix", ***Appl. Phys. Lett***. 102, 102103 (2013)

21 Y. Zhao, **Q. Yan**, D. Feezell, K. Fujito, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, S. Nakamura, "Optical polarization characteristics of semipolar (30-31) and (30-3-1) InGaN/GaN light-emitting diodes", ***Opt. Express*** 21, A53 (2013)

20 E. Kioupakis, **Q. Yan**, and C. G. Van de Walle, "Interplay of polarization fields and Auger recombination in the efficiency droop of nitride light-emitting diodes", ***Appl. Phys. Lett.*** 101, 231107 (2012)

19 M. S. Miao, **Q. Yan**, C. G. Van de Walle, W. K. Lou, L. L. Li, and K. Chang, "Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well", ***Phys. Rev. Lett.*** 109, 186803 (2012)

18 **Q. Yan**, P. Rinke, M. Scheffler, and C. G. Van de Walle, "Strain effects and band parameters in MgO, ZnO and CdO", ***Appl. Phys. Lett.*** 101, 152105 (2012)

17 Y. Kawaguchi, C. Y. Huang, Y. R. Wu, **Q. Yan**, C. C. Pan, Y. Zhao, S. Tanaka, K. Fujito, D. Feezell, C. G. Van de Walle, S. P. DenBaars, and S. Nakamura "Influence of Polarity on Carrier Transport in Semipolar Multiple-Quantum-Well (20-21) and (20-2-1) Light-Emitting Diodes", ***Appl. Phys. Lett.*** 100, 23111 (2012)
"Appl. Phys. Lett. Editor's Picks of the Year Award" in 2012.
"Research Highlights" of American Institute of Physics and Top 20 most downloaded articles on Appl. Phys. Lett. in June 2012.

16 Y. Zhao, **Q. Yan**, C. Y. Huang, S. C. Huang, P. S. Hsu, S. Tanaka, C. C. Pan, Y. Kawaguchi, K. Fujito, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, S. Nakamura, and D. Feezell, "Indium incorporation and emission properties of nonpolar and semipolar InGaN quantum wells", ***Appl. Phys. Lett.*** 100, 201108 (2012)

15 **Q. Yan**, A. Janotti, M. Scheffler, and C. G. Van de Walle, "Role of nitrogen vacancies in the luminescence of Mg-doped GaN", ***Appl. Phys. Lett.*** 100, 142110 (2012)
Top 20 most downloaded articles on Appl. Phys. Lett. in April 2012.

14 C. Roberts, **Q. Yan**, M. S. Miao, and C. G. Van de Walle, "Confinement effects on valence-subband character and polarization anisotropy in (11-22) semipolar InGaN/GaN quantum wells", ***J. Appl. Phys.*** 111, 073113 (2012);

13 C. Y. Huang, **Q. Yan**, Y. Zhao, K. Fujito, D. Feezell, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, S. Nakamura, "Influence of Mg-doped barriers on semipolar (20-21) multiple-quantum-well green light-emitting diodes", ***Appl. Phys. Lett.*** 99, 141114 (2011)

12 Y. Zhao, S. Tanaka, **Q. Yan**, C. Y. Huang, R. B. Chung, C. C. Pan, K. Fujito, D. Feezell, C. G. Van de Walle, J. S. Speck, S. P. DenBaars, and S. Nakamura, "High optical polarization ratio from semipolar (20-2-1) blue-green InGaN/GaN light-emitting diodes", ***Appl. Phys. Lett.*** 99, 051109 (2011)

11 P. G. Moses, M. S. Miao, **Q. Yan**, and C. G. Van de Walle, "Hybrid functional investigations of band gaps and band alignments for AlN, GaN, InN, and InGaN", ***J. Chem. Phys.*** 134, 084703 (2011)

10 **Q. Yan**, P. Rinke, M. Winkelnkemper, A. Qteish, D. Bimberg, M. Scheffler, and C. G. Van de Walle, "Band parameters and strain effects in ZnO and group-III nitrides", ***Semi. Sci. Tech.*** 26, 014037 (2011) *Selected as a "Highlight of 2011" in Semi. Sci. Tech.*

9 **Q. Yan**, P. Rinke, M. Scheffler, and C. G. Van de Walle, "Role of strain in polarization switching in semipolar InGaN/GaN quantum wells", ***Appl. Phys. Lett.*** 97, 181102 (2010)

8 **Q. Yan**, P. Rinke, M. Scheffler, and C. G. Van de Walle, "Strain effects in group-III nitrides: Deformation potentials for AlN, GaN, and InN", ***Appl. Phys. Lett.*** 95, 121111 (2009)

7 B. Huang, **Q. Yan**, Z. Li, W. H. Duan, "Towards graphene nanoribbon-based electronics", ***Front. Phys. China.*** 4, 269 (2009)

6 J. Yu, Z. Wu, Z. Liu, **Q. Yan**, J. Wu and W. H. Duan, "Phase diagram of ferroelectric $BaTiO_3$ ultrathin films under open-circuit conditions", ***J. Phys.: Condens. Matter*** 20, 135203 (2008)

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