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

2022- present Associate Professor,
Department of Physics, Northeastern University

2016- 2022 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, U.S. 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 CAREER Program; NSF CDS&E Program; NSF OAX SSE; NSF AI Institute, NSF Division of Materials Research; DOE BES Early Career Program; DOE Quantum Information Science Program; DOE EPSCoR Program; DOE Computational Materials Science Program Proposal review board member for the Center for Nanoscale Materials at Argonne National Laboratory.

- Referee of Physical Review Letters, Nature Communications, 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

Northeastern University

Spring 2024	Physics 2303 – Modern Physics
Spring 2023	Physics 2303 – Modern Physics

Temple University

Spring 2022	Physics 4511 - Scientific Computing III
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

Northeastern University

2024-present	Yu Ruan, Master Student
2023-present	Zhenyao Fang, Postdoc Researcher
	Ayushi Shirke, Graduate Student
2022-present	Weiyi Gong, Graduate Student
	Anoj Aryal, Graduate Student
	Alex Heilman, Graduate Student
	Claire Schlesinger, Undergraduate Co-Op student
2022-2023	Jeng-Yuan Tsai, Postdoc Researcher
	(Now as a Data Processing Scientist at Jefferson Lab)
	Yubo Qi, Associate Research Scientist
	(Now as an Assistant Professor at University of Alabama)

Temple University

2021-2022	Anoj Aryal, Graduate Student
	Alex Heilman, Graduate Student
2021-2022	Debajit Chakraborty, Research Assistant Professor
2020-2022	Andy Philips, Undergraduate Student
2020-2021	Brendan Magdamo, Undergraduate Student
2019-2022	Weiyi Gong, Graduate Student
2019-2020	Lifu Zhang, Visiting Student
2019 summer	Francesco Ricci, Visiting Scholar
2018-2022	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 Associate Professor at University of Central Florida)

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

Invited Presentations

1. GRC Conference for Defects in Semiconductors, Newry, MN (August 2024)
   Symmetry-guided and machine learning assisted design of quantum defects in 2D materials
2. AI Retreat, University of Alabama, Birmingham, AL (January 2024)
   Physical principle informed AI and machine learning for science and engineering problems
3. Condensed Matter Seminar, Boston University, Boston, MA (November 2023)
   Data-driven materials design in the quantum regime
4. NST Colloquium, Argonne National Laboratory, Chicago, IL (October 2023)
   Machine learning in the quantum regime through physical-principle-informed representations
5. International Conference on Defects in Semiconductors, Rehoboth Beach, DE (Sept 2023)
   Data-driven discovery and design of quantum defects in 2D materials
6. 50 years of DFT, Celebration of John Perdew's 80th birthday, New Orleans, LA (June 2023)
   Incorporation of density scaling constraint in density functional design via contrastive learning
7. Materials-2023 workshop, Houston, Texas (April 2023)
   Symmetry-enabled data-driven design of quantum defects in 2D materials
8. MRS Spring Meeting, San Francisco, CA (April 2023)
   Machine learning in the quantum regime through physical-principle-informed representations
9. PCSI-48 workshop, Redondo Beach, CA (January 2023)
   Machine learning in the quantum regime through physical-principle-informed representations
10. Condensed Matter Seminar, University of Texas, Austin, TX (November 2022)
    Machine learning in the quantum regime through physical-principle-enabled representation learning
11. Joint Colloquium, Colleges of Science and Engineering, Northeastern University, MA (April 2022)
    Data-driven materials design in the quantum regime
12. Materials-2022 workshop, Newton, MA (April 2022)
    Quantum defects in two dimensional materials: local-symmetry-guided discovery and design
13. Department Colloquium, Department of Physics, University of Florida, FL (Jan. 2022)
    Data-driven materials design in the quantum regime: motif centric learning and symmetry-guided materials discovery
14. Condensed Matter Seminar, Stony Brook University, NY (2021)
    Data-driven materials design in the quantum regime
15. Department of Materials Science and Engineering, University of Pennsylvania, PA (2021)
    Data-driven materials design in the quantum regime
16. Physics Colloquium, Temple University, Philadelphia, PA (2020)

Symmetry enabled effective learning and accelerated discovery of quantum materials

17. SCAN Workshop, Temple University, Philadelphia, PA (2019)

    Data-driven discovery of functional 2D materials using a SCAN-enabled electronic structure database

18. Department of Physics, Penn State University, University Park, PA (2018)

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

19. Lecture Series on Materials Theory and Computation, Xi'an, China (2018)

    Data-driven discovery of functional 2D materials

20. Department of Applied Physics & Materials, California Institute of Technology, CA (2018)

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

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

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

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

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

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

    Data-driven discovery of solar fuels photoanode materials

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

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

25. 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

26. 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
27. Beijing Computational Science Research Center, Beijing, China (2017)
    Materials Genome Initiative and data-driven discovery of solar fuels photoanode materials
28. Electronic Materials and Applications 2017, Orlando, FL (2017)

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

29. 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
30. 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

31. 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

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

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

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

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

34. 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

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

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

36. Department of Materials Science and Engineering, Shanghai Jiaotong University, China (2015)

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

37. Materials Genome Institute, Shanghai University, China (2015)

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

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

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

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

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

40. 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

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

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

42. 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

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

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

44. 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

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

    Electronic structure and transport property of carbon ribbons

Publications

89 scientific publications; **2** U.S. patents; **1** book chapter.

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

Total citations: **6745**; h-index: **41**; **21** publications with over 100 citations.

89 Z. Fang, **Q. Yan**, "Leveraging Persistent Homology Features for Accurate Defect Formation Energy Predictions via Graph Neural Networks", arXiv:2407.05204 (2024), DOI: 10.48550/arXiv.2407.05204

88 Y. Qi, W. Gong, **Q. Yan**, "Bridging deep learning force fields and electronic structures with a physics-informed approach", arXiv:2403.13675 (2024), DOI: 10.48550/arXiv.2403.13675

87 A. Heilman, C. Schlesinger, **Q. Yan**, "Equivariant Graph Neural Networks for Prediction of Tensor Material Properties of Crystals", arXiv:2406.03563 (2024), DOI: 10.48550/arXiv.2406.03563

86 J. Y. Tsai, W. Gong, **Q. Yan**, "Symmetry-guided data-driven discovery of native quantum defects in two-dimensional materials", arXiv:2405.11379 (2024), DOI: 10.48550/arXiv.2405.11379

85 Z. Fang, **Q. Yan**, "Towards accurate prediction of configurational disorder properties in materials using graph neural networks", ***npj Computational Materials*** 10, 91 (2024), DOI: 10.1038/s41524-024-01283-w

84 Z. Wang, Y. Huang, W. Gong, **Q. Yan**, S. Ren, "Lithiation bridged molecular conducting magnets", ***Applied Materials Today*** 38, 102188 (2024), DOI: 10.1016/j.apmt.2024.102188

83 Z. Wang, Q. Wang, W. Gong, A. Chen, A. Islam, L. Quan, T. J. Woehl, Q. Yan, S. Ren, "Magnet-in-ferroelectric crystals exhibiting photomultiferroicity", ***PNAS*** 121, e2322361121 (2024), DOI: 10.1073/pnas.2322361121

82 G. Kim, B. Huet, C. E. Stevens, K. Jo, J.-Y. Tsai, S. Bachu, M. Leger, K. Y. Ma, N. R. Glavin, H. S. Shin, N. Alem, **Q. Yan**, J. R. Hedrickson, J. M. Redwing, D. Jariwala, "Exciton Confinement in Two-Dimensional, In-Plane, Quantum Heterostructures", ***Nature Communications*** 15, 6361 (2024), DOI: 10.1038/s41467-024-50653-x

81 Q Gao, **Q Yan**, Z Hu, L Chen "Bilayer Kagome Borophene with Multiple van Hove Singularities", ***Adv. Sci.*** 202305059 (2023)

80 **Q. Yan**, S. Chowdhury, A. Bansil, S. Kar, "The Case for a Defect Genome Initiative", ***Adv. Mater.*** 2303098 (2023). DOI: 10.1002/adma.202303098

79 W. Gong, T. Sun, H. Bai, P. Chu, A. Aryal, J. Yu, H. Ling, J. P. Perdew, **Q. Yan**, "Incorporation of density scaling constraint in density functional design via contrastive representation learning", ***Digital Discovery*** 2, 1404 (2023). DOI: 10.1039/D3DD00114H

78 Y. Huang, A. Pathak, C. Rumsey, N. Kramer, Y. Hu, M. Trebbin, J.-Y. Tsai, M. Ivill, **Q. Yan**, S. Ren, "Pressure-Controlled Magnetism in 2D Molecular Layers", ***Nature Commun.*** 14, 3186 (2023). DOI: 10.1038/s41467-023-38991-8

77 S. Singh, W. Gong, C. Stevens, J. Hou, A. Mohite, J. Hendrickson, **Q. Yan**, D. Jariwala, "Valley Polarized Interlayer Excitons in 2D Chalcogenide-Halide Perovskite-Van der Waals Heterostructures", ***ACS Nano*** 17, 7487 (2023), DOI: 10.1021/acsnano.2c12546

76 C. Becher, W. Gao, S. Kar, C. Marciniak, T. Monz, J. G. Bartholomew, P. Goldner, H. Loh, E. Marcellina, K. E. J. Goh, T. S. Koh, B. Weber, Z. Mu, J.-Y. Tsai, **Q. Yan**, S. Gyger, S. Steinhauer, V. Zwiller, "2023 Roadmap for Materials for Quantum Technologies", ***Mater. Quantum. Technol.*** 3, 012501 (2023), DOI: 10.1088/2633-4356/aca3f2

75 H. Tang, S. Neupane, **Q. Yan**, A. Ruzsinszky, "Density Functional Theory Study of Controllable Optical Absorptions and Magneto-Optical Properties of Magnetic CrI3 Nanoribbons: Implications for Compact 2D Magnetic Devices", ***ACS Appl. Nano Mater.*** 5, 14388 (2022), DOI: 10.1021/acsanm.2c02722

74 Y. Huang, W. Gong, G. Zhang, Z. Li, H. Lin, **Q. Yan**, S. Ren, "Dimensional Transformation of Molecular Magnetic Materials" ***ACS Nano*** 16, 13232 (2022), DOI: 10.1021/acsnano.2c06912

73 J.-Y. Tsai, J. Pan, H. Lin, A. Bansil, **Q. Yan**, "Antisite defect qubits in monolayer transition metal dichalcogenides", ***Nat. Commun.*** 13, 492 (2022), DOI: 10.1038/s41467-022-28133-x

72 Y. Hu, W. Gong, S. Wei, S. Khuje, Y. Huang, Z. Li, Y. C. Li, F. Yao, **Q. Yan**, S. Ren, "Lithiating Magneto-Ionics in Rechargeable Battery" ***PNAS*** 119, e2122866119 (2022), DOI: 10.1073/pnas.2122866119

71 A. Sheng, S. Khuje, J. Yu, T. Parker, J.-Y. Tsai, L. An, Y. Huang, Z. Li, C.-G. Zhuang, L. Kester, **Q. Yan**, S. Ren, "Copper Nanoplates for Printing Flexible High-Temperature Conductors"**. *ACS Appl. Nano Mater.*** 5, 4028 (2022), DOI: 10.1021/acsanm.2c00019

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.*** 34, 4625 (2022), DOI: 10.1007/s00521-021-06616-0

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. Mater.*** 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)

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