Yuanxi Wang

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Education

2016 Ph.D. in Phyiscs, Pennsylvania State University (Mentor: Vincent H. Crespi)
2010 B.Sc. in Physics, Kuang Yaming Honors School, Nanjing University, China

Research and Professional experience

2021-	Assistant Professor, Department of Physics, University of North Texas
2018-2021	Assistant Research Professor, 2-Dimensional Crystal Consortium, Material Research Institute, Pennsylvania State University
2017-2018	Research Associate, 2-Dimensional Crystal Consortium, Material Research Institute, Pennsylvania State University
2016-2017	Postdoctoral Scholar, 2-Dimensional Crystal Consortium, Material Research Institute, Pennsylvania State University
2012-2016	Research Assistant, Physics Department, Pennsylvania State University
2010-2012	Graduate Assistant, Physics Department, Pennsylvania State University
2009-2010	Research Assistant, exchange program, University of California Los Angeles

Research Areas

Condensed matter theory of low-dimensional materials with emphasis on:

- Excited-state materials properties from many-body perturbation theory
- Theory of defects and 2D growth kinetics
- Electronic structure and transport properties from first-principles computation

Grant Awards

- **Awarded as PI or Co-PI**

2022 University of North Texas Advanced Materials and Manufacturing Processes Institute Seed Grant, $6,000, PI
2022 University of North Texas College of Science Seed Grant, $10,000, PI
2022 ORNL Center for Nanophase Materials Sciences User proposal "Transfer learning methods and advanced first-principles methods in modeling point defects", 501,000 CPU hours award at NERSC, PI
2022 Penn State 2DCC User Proposal R0076 "Nonlinear optical response in 2D layered materials", 500,000 CPU hours, PI
2021 TACC-DMR21025 "First-principles theory modeling of defects and nonlinear optical response in 2D materials", 256,000 CPU hours awarded on TACC-Lonestar6, PI
2020 NSF XSEDE Allocation TG-DMR170050 "Simulated synthesis and characterization of 2D chalcogenides from first-principles", 800,000 CPU hours awarded on TACC-Stampede2, PI
2018 NSF XSEDE Allocation TG-DMR170050 "Simulated synthesis and characterization of 2D chalcogenides from first-principles", 420,000 CPU hours awarded on TACC-Stampede2, PI
2017 NSF XSEDE Allocation TG-DMR170050 "Simulated synthesis and characterization of 2D chalcogenides from first-principles", 420,000 CPU hours awarded on LSU-superMIC ($28,190.40 equivalent), co-PI

- **Awarded as Senior research personnel**

2021 NSF Partnership for Research and Education in Materials award, a PSU-FIU partnership, $3,780,000

2020 Renewal for the PSU Center for Nanoscale Science, a Materials Science and Engineering Center, "Interdisciplinary Research Group (IRG) 1: 2D Polar Metals and Heterostructures", total amount for two IRGs $3,590,000

2018 Supplement to NSF PREM Award DMR-1205734 in collaboration with CalState Northridge, "Data-driven Discovery of Novel 2D Materials for Optoelectronic Applications", total amount $100,000, PSU amount $40,000

2018 Supplement to NSF 2DCC-MIP Award DMR-1539916 in collaboration with Iowa State University and University of Florida, "High-throughput identification of Incipient 2D Materials" and "Data-driven Synthesizability Assay for 2D Materials", $500,000

Honors & Awards

2022 UNT D.C. Faculty Research Fellow

2012 Duncan Fellowship in Physics

2010 Elsbach Distinguished Graduate Fellowship

2010 Braddock Scholarship

Publications

~2100 citations from Google Scholar (∗= equal contribution, †= corresponding author)

39. **Y. Wang**, P. Lammert, V. H. Crespi, M. L. Cohen, A. Nourhani, "Non-stoichiometric salt intercalation of bilayer graphene", Phys. Rev. Lett. **129**, 266401 (2022)
38. H. Yi*, L.-H. Hu*, **Y. Wang***, R. Xiao, J. Cai, D. R. Hickey, C. Dong, Y.-F. Zhao, L.-J. Zhou, R. Zhang, A. R. Richardella, N. Alem, J. A. Robinson, M. H. W. Chan, X. Xu, N. Samarth, C.-X. Liu, and C.-Z. Chang, "Crossover of Ising- to Rashba-Type Superconductivity in Epitaxial Bi_2Se_3/Monolayer $NbSe_2$ Heterostructures", Nat. Mater. **21**, 1366 (2022)
37. K. Yang, **Y. Wang**, C.X. Liu, "Momentum-space Spin Anti-vortex and Spin Transport in Monolayer Pb", Phys. Rev. Lett. **128**, 166601 (2022)
36. W. Lee, **Y. Wang**, H. Kim, M. Liu, T. N. Nunley, B. Fang, R. Maniyara, C. Dong, J. A. Robinson, V. Crespi, X. Li, A. H. MacDonald, and C.-K. Shih, "Confined monolayer Ag as a large gap 2D semiconductor and its many-body interactions with high-density Dirac electrons", Nano Lett. **22**, 7841 (2022)
35. J. He, S. H. Lee, F. Naccarato, G. Brunin, R. Zu, **Y. Wang**, L. Miao, H. Wang, N. Alem, G. Hautier, G.-M. Rignanese, Z. Mao, and V. Gopalan, "SnP_2S_6: A Promising Infrared Nonlinear Optical Crystal with Strong Nonresonant Second Harmonic Generation and Phase-Matchability", ACS Photonics, **9**, 1724 (2022)
34. Q. Qian, W. Wu, L. Peng, **Y. Wang**, A. M. Z. Tan, L. Liang, S. M. Hus, K. Wang, T. H. Choudhury, J. M. Redwing, A. A. Puretzky, D. B. Geohegan, R. G. Hennig, X. Ma, and S. Huang, "Photoluminescence Induced by Substitutional Nitrogen in Single-Layer Tungsten Disulfide", ACS Nano **16**, 7428 (2022)
33. Y. Lin†, E. Hathaway, F. Habis, **Y. Wang**†, R. G. Rodriguez, K. Alnasser, N. Hurley, J. Cui, "Enhanced Emission from Defect Levels in Multilayer MoS_2", Adv. Optical Mater. **10**, 2201059 (2022)
32. **Y. Wang**, "Chemical requirements for stabilizing type-II Weyl points in $MnBi_{2-x}Sb_xTe_4$", arXiv:2103.12730
31. S. H. Lee, D. Graf, L. Min, Y. Zhu, H. Yi, S. Ciocys, **Y. Wang**, E. S. Choi, R. Basnet, A. Fereidouni, A Wegner, Y. Zhao, K. Verlinde, J. He, R. Redwing, V. Gopalan, H. O. H. Churchill, A. Lanzara, N. Samarth, C.-Z. Chang, J. Hu and Z.Q. Mao "Evidence for a magnetic-field induced ideal type-II Weyl state in antiferromagnetic topological insulator $Mn(Bi_{1-x}Sb_x)_2Te_4$", Phys. Rev. X **11**, 031032 (2021)
30. **Y. Wang**, V. H. Crespi, "Atlas of 2D metals epitaxial to SiC: filling-controlled gapping conditions and alloying rules", arxiv:2011.01914

29. M. A. Steves, **Y. Wang**, N. Briggs, T. Zhao, H. El-Sherif, B. Bersch, S. Subramanian, C. Dong, T. Bowen, A. De La F. Duran, K. Nisi, M. Lassauniere, U. Wurstbauer, N. Bassim, J. J. Fonseca, J. T. Robinson, V. H. Crespi, J. A. Robinson, K. L. Knappenberger, Jr., "Unexpected Near-Infrared to Visible Non-linear Optical Properties from Two-Dimensional Polar Metals", Nano Lett. **20**, 8312 (2020)
28. Y. Sun, **Y. Wang**, J. Y. C. Chen, K. Fujisawa, J. T. Miller, V. H. Crespi, M. Terrones, R. E. Schaak, "Interface-mediated noble metal deposition on transition metal dichalcogenide nanostructures", Nat. Chem. **12**, 284 (2020)
27. N. Briggs*, B. Bersch*, **Y. Wang***, J. Jiang, R. J. Koch, N. Nayir, K. Wang, M. Kolmer, W. Ko, A. D. L. F. Duran, S. Subramanian, C. Dong, J. Shallenberger, M. Fu, Q. Zou, Y.-W. Chuang, Z. Gai, A.-P. Li, A. Bostwick, C. Jozwiak, C.-Z. Chang, E. Rotenberg, J. Zhu, A. C. T. van Duin, V. H. Crespi, and J. A. Robinson, "Atomically Thin, Half-van der Waals Materials enabled by Confinement Heteroepitaxy", Nat. Mater. **19**, 637 (2020)
26. F. Zhang, B. Zheng, A. Sebastian, H. Olson, M. Liu, K. Fujisawa, Y. T. H. Pham, V. O. Jimenez, V. Kalappattil, L. Miao, Tianyi Zhang, Rahul Pendurthi, Y. Lei, A. L. Elías, **Y. Wang**, N. Alem, P. E. Hopkins, S. Das, V. H. Crespi, M.-H. Phan , M. Terrones, "Monolayer Vanadium-doped Tungsten Disulfide: A Room-Temperature Dilute Magnetic Semiconductor", Adv. Sci. **7**, 2001174 (2020)
25. N. Nayir, **Y. Wang**, S. Shabnam, D. Hickey, L. Miao, X. Zhang, S. Bachu, N. Alem, J. Redwing, V. Crespi, A. van Duin, "Modeling for Structural Engineering and Synthesis of Two Dimensional WSe_2 Using a Newly Developed ReaxFF Reactive Force Field", J. Phys. Chem. C **124**, 51 (2020)
24. K. Momeni, Y. Ji, **Y. Wang**, S. Paul, S. Neshani, D. E. Yilmaz, Y. K. Shin, D. Zhang, J.-W. Jiang, H. S. Park, S. Sinnott, A. van Duin, V. H. Crespi, L.-Q. Chen, "Computational Synthesis of 2D Materials Beyond Graphene: A Review", npj Comput. Mater. **6**, 22 (2020)
23. K. Zhang D. D. Deng, B. Zheng, **Y. Wang**, F. K. Perkins, N. C. Briggs, V. H. Crespi, J. A. Robinson, "Tuning Transport and Chemical Sensitivity via Niobium Doping of Synthetic MoS_2", Adv. Mater. Interfaces 2000856 (2020)
22. X. Zhang*****, F. Zhang*****, **Y. Wang**, D. S. Schulman, T. Zhang, A. Bansal, N. Alem, S. Das, V. H. Crespi, M. Terrones, J. M. Redwing, "Defect-controlled nucleation and orientation of WSe_2 on hBN – a route to single crystal epitaxial monolayers", ACS Nano **13**, 3341 (2019).
21. F. Zhang*****, **Y. Wang***†, C. Erb, K. Wang, P. Moradifar, V. H. Crespi†, N. Alem†, "Full orientation control of epitaxial MoS_2 on hBN assisted by substrate defects", Phys. Rev. B **99**, 155430 (2019)
20. **Y. Wang**†, B. R. Carvalho, V. H. Crespi†, "Strong exciton regulation of Raman scattering in monolayer MoS_2", Phys. Rev. B (Rapid Commun.) **98**, 161405 (2018)
19. B. R. Carvalho, **Y. Wang**, K. Fujisawa, T. Zhang, V. H. Crespi, M. A. Pimenta, M. Terrones, L. M. Malard, "Nonlinear dark-field imaging of 1D defects in monolayer dichalcogenides", Nano Lett. **20**, 284, (2020)
18. S. Subramanian, K. Xu, **Y. Wang**, S. Moser, N. A. Simonson, D. Deng, V. H. Crespi, S. K. Fullerton-Shirey, J. A. Robinson, "Tuning transport across MoS_2/graphene interfaces via as-grown lateral heterostructures", npj 2D Mater. Appl. **4**, 9 (2020)
17. R. Rao, V. Carozo, **Y. Wang** , A. E. Islam, N.P.-Lopez, K. Fujisawa, V. H. Crespi, M.Terrones, B. Maruyama, "Cleaning, Passivating and Doping Monolayer MoS_2 by Controlled Laser Irradiation", 2D Mater. 6, 045031 (2019)
16. Y. Xuan, A. Jain, S. Zafar, R. Lotfi, N. Nayir, **Y. Wang**, T. H. Choudhury, S. Wright, J. Feraca, L. Rosenbaum, J. M. Redwing, V. H. Crespi, A. van Duin, "Multi-scale modeling of gas-phase reactions in metal-organic chemical vapor deposition growth of WSe_2", J. Cryst. Growth 527, 125247 (2019).
15. K. Zhang, **Y. Wang**, J. Joshi, F. Zhang, S. Subramanian, M. Terrones, P. Vora, V. H. Crespi, J. A. Robinson, "Probing the lateral heterogeneities in synthetic monolayer molybdenum disulfide", 2D Mater. **6**, 025008 (2019)

14. Z. Zhang*, **Y. Wang***, X. Leng, V. H. Crespi, F. Kang, R. Lv, "Controllable Edge Exposure of MoS_2 for Efficient Hydrogen Evolution with High Current Density", ACS Appl. Energy Mater. **1**, 1268 (2018)
13. Z. Lin *et al.*, "Recent Progress on 2D Materials Beyond Graphene: From Ripples, Defects , Intercalation, and Valley Dynamics, to Straintronics, and Power Dissipation", APL Mater. **6**, 080701 (2018)
12. **Y. Wang**, V. H. Crespi, "Nanovelcro: Theory of guided folding in atomically thin sheets with regions of complementary doping", Nano Lett. **17**, 6708 (2017)
11. **Y. Wang** and V. H. Crespi, "Theory of Finite-length Grain Boundaries of Controlled Misfit Angle in Two-dimensional Materials", Nano Lett. **17**, 5297 (2017)
10. A. McCreary, J. Simpson, **Y. Wang**, D. Rhodes, K. Fujisawa, L. Balicas, M. Dubey, V. H. Crespi, M. Terrones, A. R. H. Walker, "Intricate Resonant Raman Response in Anisotropic ReS_2, Nano Lett. **17**, 5897 (2017)
9. A. Azizi, **Y. Wang**, G. Stone, A. L. Elías, Z. Lin, M. Terrones, V. H. Crespi and N. Alem, "Defect Coupling and Sub-Ångstrom Structural Distortions in $W_{1-x}Mo_xS_2$ Monolayers", Nano Lett. **17**, 2802 (2017)
8. V. Carozo, **Y. Wang**, K. Fujisawa, B. R. Carvalho, A. McCreary, S. Feng, Z. Lin, C. Zhou, N. P.-López, A. L. Elías, B. Kabius, V. H. Crespi, M. Terrones, "Optical identification of sulfur vacancies: Bound excitons at the edges of monolayer tungsten disulfide", Sci. Adv, **3** (4), e1602813 (2017)
7. B. R. Carvalho*, **Y. Wang***, L. M. Malard, S. Mignuzzi, D. Roy, M. Terrones, C. Fantini, V. H. Crespi, M. A. Pimenta, "Intervalley scattering by acoustic phonons in two-dimensional MoS_2 revealed by double-resonance Raman spectroscopy", Nat. Commun. **8**, 14670 (2017)
6. A. Ostadhossein, A. Rahnamoun, **Y. Wang**, P. Zhao, S. Zhang, V. H. Crespi, A. C. T. van Duin, "ReaxFF Reactive Force-Field Study of Molybdenum Disulfide (MoS_2)", J. Phys. Chem. Lett. **8** (3), 631-640 (2017)
5. A. Azizi, **Y. Wang**, Z. Lin, K. Wang, M. Terrones, V. H. Crespi, N. Alem, "Spontaneous formation of atomically thin stripes in transition metal dichalcogenide monolayers", Nano Lett. **16**, 6982 (2016)
4. Y. Sun, **Y. Wang**, D. Sun, B. R. Carvalho, C. G. Read, C.-H. Lee, Z. Lin, K. Fujisawa, J. A. Robinson, V. H. Crespi, M. Terrones, R. E. Schaak, "Low-Temperature Solution Synthesis of Few-Layer 1T′-$MoTe_2$ Nanostructures Exhibiting Lattice Compression," Angew. Chem. Int. Ed. **55** (8), 2830 (2016)
3. N. I. Kovtyukhova, **Y. Wang**, A. Berkdemir, R. Cruz-Silva, M. Terrones, V. H. Crespi, T. E. Mallouk, "Nonoxidative intercalation and exfoliation of graphite by Brønsted acids", Nat. Chem. **6**, 957 (2014) (cover article)
2. C. Janisch, **Y. Wang**, D. Ma, N. Mehta, A. L. Elías, N. P.-López, M. Terrones, V. H. Crespi, Z. Liu, "Extraordinary Second Harmonic Generation in Tungsten Disulfide Monolayers", Sci. Rep. **4**, 5530 (2014)
1. N. I. Kovtyukhova, **Y. Wang**, R. Lv, M. Terrones, V. H. Crespi, T. E. Mallouk, "Reversible Intercalation of Hexagonal Boron Nitride with Brønsted Acids", J. Am. Chem. Soc. **135** (22), 8372-8381 (2013)

Invited talks

- Graphene and Beyond Workshop, "Why crystalize in layers: Design principles for layered nonlinear optical crystals", May 2022
- University of Arkansas, Physics colloquium, Oct 2021
- Florida International University, MRS Student Chapter Webinar, Jul 2021
- California State University Northridge, Physics colloquium, May 2021
- University of California San Diego, Physical chemistry seminar, Feb 2020
- APS March Meeting 2020, "Defect-enabled high crystallinity in 2D semiconductors and heterostructures", R57.00007

- Graphene and Beyond Workshop 2019, "Localized strong couplings in 2D materials"
- Penn State 2DCC Invited Webinar, Jan 2018, "Modeling 2D Growth outcomes"

Contributed talks

- APS March Meeting 2022, "Stability of type-II Weyl points in $MnBi_{2-x}Sb_xTe_4$ based on orbital interactions"
- APS March Meeting 2021, "Atlas of air-stable 2D metals: gapping conditions, alloying rules, and superconductivity"
- MRS Fall Meeting 2020, "Atlas of 2D Metals Epitaxial to SiC: Gapping Conditions and Alloying Rules", F.EL04.08.07, (link to recorded talk)
- APS March Meeting 2019, "Exciton regulation of resonant Raman scattering in monolayer MoS_2"
- APS March Meeting 2018, "Epitaxial MoS_2 on h-BN without mirror grain boundaries"
- APS March Meeting 2017, "Resonance Raman intensities including excitonic effects from first-principles: application to 2D materials"
- APS March Meeting 2017, "Bound excitons at the edges in monolayer WS_2"
- APS March Meeting 2016, "Intervalley double resonance processes in MoS_2"
- APS March Meeting 2015, "Structural and transport properties of finite length grain boundaries in two-dimensional materials"
- APS March Meeting 2014, "The formation and pinning of folds in 2D materials"
- APS March Meeting 2013, "Morphology control of WS_2 monolayer islands"

Teaching

- Spring 2023, Phys 3910, Intermediate Computational Modeling of Physical Systems
- Fall 2022, Phys 3510, Physics, Computation and Software Applications
- Spring 2022, Phys 4110, Statistical and Thermal Physics
- Spring 2019, Guest lectures, PSU Phys 514, Physics of surfaces, interfaces, and thin films

Collaborators and affiliations

Anupama Kaul (UNT 2022), Yuankun Lin (UNT 2022), Jingbiao Cui (UNT 2022), Chaoxing Liu (PSU 2021), Zhiqiang Mao (PSU 2021), Daniela Radu (FIU 2021), Richard Hennig (UFl 2020), Cui-Zu Chang (PSU 2020), Venkatraman Gopalan (PSU 2020), Shengxi Huang (PSU 2020), Kenneth Knappenberger Jr (PSU 2019), Jun Zhu (PSU 2019), Joan Redwing (PSU 2018), Joshua Robinson (PSU 2018), Angela Walker (NIST 2017), Benji Maruyama (AFRL 2017), Sulin Zhang (PSU 2017), Nasim Alem (PSU 2015), Adri van Duin (PSU 2013), Zhiwen Liu (PSU 2014), Thomas Mallouk (PSU 2013), Leandro Malard (UFMG 2016), Marcos Pimenta (UFMG 2016), Raymond Schaak (PSU 2015), Mauricio Terrones (PSU 2013).

Mentoring

- Postdoc advised: Bimal Neupane (UNT, 2022-present)
- PhD Students advised: Bhojraj Bhandari (UNT), Fatimah Habis (UNT), Leticia Damian (UNT), Trace Bivens (UNT).
- PhD Students co-advised: Roberto Prado-Rivera (Florida International U), Boyang Zheng (PSU), Benjamin Katz (PSU)
- Undergraduate and UNT TAMS students advised: Eric Peng, Nehal Singh, Victor Lin.

Professional & Outreach Activities

- Journal Referee : *Nature Communications*, *Nano Letters*, *ACS Nano*, *Physical Review Materials*, *Physical Review B*, *The Journal of Physical Chemistry*, *Chemistry of Mate-*

rials, *ACS Applied Materials & Interfaces*, *Carbon*, *2D Materials*, *Nanoscale*, *Small*, *npj Computational Materials*, *AIP Advances*, *Journal of Applied Physics*, *Scientific Reports*

- Grant Reviewer: American Chemical Society Petroleum Research Fund
- Texas Academy of Mathematics and Science (TAMS) Program (Summer 2022 – present): Advise 3 high school students in conducting research. Individual and group meetings held weekly with all TAMS students. Interim research products presented at UNT AI/CS Summer Research Program poster session.
- Fort Worth Museum of Science and History, Infinity Festival UNT Day (Nov 2022): Developed and presented virtual reality demonstration of molecular dynamics and crystal structures to museum visitors.
- Faculty advisor for UNT Women in Physics Group Grant (submitted Dec 2022)