

# Yuanxi Wang

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## EDUCATION

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2016 Ph.D. in Physics, Pennsylvania State University (Mentor: Vincent H. Crespi)

2010 B.Sc. in Physics, Kuang Yaming Honors School, Nanjing University, China

## RESEARCH AND PROFESSIONAL EXPERIENCE

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2018- 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

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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

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### • PI or Co-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

### • Senior research personnel

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

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- 2012 Duncan Fellowship in Physics
- 2010 Elsbach Distinguished Graduate Fellowship
- 2010 Braddock Scholarship

## PUBLICATIONS

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~1300 citations from [Google Scholar](#) (\*= equal contribution)

- 32. **Y. Wang**, “Chemical requirements for stabilizing type-II Weyl points in  $\text{MnBi}_{2-x}\text{Sb}_x\text{Te}_4$ ”, [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  $\text{Mn}(\text{Bi}_{1-x}\text{Sb}_x)_2\text{Te}_4$ ”, under review at Phys. Rev. X
- 31. **Y. Wang**, V. H. Crespi, “Atlas of 2D metals epitaxial to SiC: filling-controlled gapping conditions and alloying rules”, [arxiv:2011.01914](#)
- 30. 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)
- 29. 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)
- 28. 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)
- 27. 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)
- 26. 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  $\text{WSe}_2$  Using a Newly Developed ReaxFF Reactive Force Field”, J. Phys. Chem. C **124**, 51 (2020)
- 25. 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)
- 24. 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  $\text{MoS}_2$ ”, Adv. Mater. Interfaces 2000856 (2020)
- 23. 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  $\text{WSe}_2$  on hBN – a route to single crystal epitaxial monolayers”, ACS Nano **13**, 3341 (2019).
- 22. **Y. Wang**, P. Lammert, V. H. Crespi, M. L. Cohen, A. Nourhani, “Non-stoichiometric salt intercalation of bilayer graphene”, under review at Phys. Rev. Lett.

21. F. Zhang\*, **Y. Wang\***, C. Erb, K. Wang, P. Moradifar, V. H. Crespi, N. Alem, "Full orientation control of epitaxial MoS<sub>2</sub> 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<sub>2</sub>", *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<sub>2</sub>/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<sub>2</sub> 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<sub>2</sub>", *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<sub>2</sub> 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<sub>2</sub>", *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<sub>1-x</sub>Mo<sub>x</sub>S<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub>)", *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<sub>2</sub> 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, “Non-oxidative 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)

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#### INVITED TALKS

- 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 2-Dimensional Crystal Consortium Invited Webinar, Jan 2018, “Modeling 2D Growth outcomes”
- PSU 2DLM Seminar, Apr 2019, “Superconductivity in atomically thin Gallium”
- PSU 2DLM Seminar, Oct 2018, “Equilibrium at the growth edge”,
- PSU 2DLM Seminar, Sep 2017, “Twin-free growth of monolayer MoS<sub>2</sub> on hBN”

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#### CONTRIBUTED TALKS

- 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<sub>2</sub>”
- APS March Meeting 2018, “Epitaxial MoS<sub>2</sub> 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<sub>2</sub>”
- APS March Meeting 2016, “Intervalley double resonance processes in MoS<sub>2</sub>”
- 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<sub>2</sub> monolayer islands”

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#### TEACHING

- Spring 2019, Guest lectures, PSU Phys 514, Physics of surfaces, interfaces, and thin films
- Spring 2020, Participation in Instructional Foundations Series (semester-long workshop), Penn State Schreyer Institute for Teaching Excellence

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#### COLLABORATORS AND AFFILIATIONS

Zhiqiang Mao (PSU 2021), Richard G. Hennig (U Florida 2020), Cui-Zu Chang (PSU 2020), Venkat Gopalan (PSU 2020), Shengxi Huang (PSU 2020), Kenneth L. Knappenberger Jr (PSU 2019), Jun Zhu (PSU 2019), Joan M. Redwing (PSU 2018), Joshua A. Robinson (PSU 2018), Angela R. H. 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 E. Mallouk (PSU 2013), Leandro M. Malard (UFMG 2016), Marcos Pimenta (UFMG 2016), Raymond E. Schaak (PSU 2015), Mauricio Terrones (PSU 2013).

## STUDENTS ADVISED AND CO-ADVISED

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Boyang Zheng (PSU), Benjamin Katz (PSU), Roberto Prado-Rivera (Florida International U)

## PROFESSIONAL ACTIVITIES

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Referee for the following journals: *Nature Communications*, *Nano Letters*, *ACS Nano*, *Physical Review Materials*, *Physical Review B*, *The Journal of Physical Chemistry*, *Chemistry of Materials*, *ACS Applied Materials & Interfaces*, *Carbon*, *2D Materials*, *Nanoscale*, *Small*, *npj Computational Materials*, *AIP Advances*, *Journal of Applied Physics*, *Scientific Reports*