Curriculum Vitae

John Villanova

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Education

- Ph.D. Physics (Condensed Matter Theory), Virginia Polytechnic Institute and State University (Virginia Tech) — May 2018
  Advisor: Dr. Kyungwha Park
- B.S. Physics (summa cum laude), Appalachian State University — May 2013

Research Experience

- Oct. 2021 – Present — Postdoctoral Research Associate, Oak Ridge National Laboratory, Oak Ridge, TN
  Advisor: Dr. Tom Berlijn
  - Derived magnetic interactions from first-principles in quantum spin liquid candidate materials in collaboration with experimentalists
  - Created a new theoretical formalism to derive magnetic form factors of quantum materials from first principles
  - Led a combined theoretical and experimental study of the electronic structure of the kagome charge density wave material ScV6Sn6, including creating analysis programs to interpret scanning tunneling microscopy data

- Aug. 2018 – Sept. 2021 — Postdoctoral Research Associate, University of Arkansas, Fayetteville, AR
  Advisor: Dr. Salvador Barraza-Lopez
  - Investigated the structural phase transformation and thermoelectric properties of two-dimensional ferroelectric monochalcogenide monolayers
  - Calculated phonon dispersions from finite differences on supercells and separately from the velocity autocorrelation function
  - Performed peak analysis on the phonon density of states spectrum to develop an in-house method of extracting the phonon lifetime, lattice thermal conductivity, and then electronic contributions to thermoelectricity in SnSe

- May 2014 – July 2018 — Graduate Research Assistant, Virginia Tech, Blacksburg, VA
  Advisor: Dr. Kyungwha Park
  - Performed density functional theory calculations to investigate the electronic structure and spin texture of surface states of topological insulators and Dirac and Weyl semimetals

  - Built a Wannier-function-based tight-binding model for topological materials from DFT calculations and continuing to study their topological properties under applied strain and magnetic field

- May 2012 – Aug. 2012 Summer Undergraduate Research Fellow, National Institute of Standards and Technology (NIST), Gaithersburg, MD
  Advisor: Mr. Xiaoyu Alan Zheng
  - Improved a visual basic profile topography correlation program by adding batch processing and iterative functions.
  - Performed a consecutively-manufactured chisel toolmark study.

- May 2011 – Aug. 2011 Summer Undergraduate Research Fellow, National Institute of Standards and Technology (NIST), Gaithersburg, MD
  Advisor: Dr. Theodore Vorburger
  - Assisted with the standard casings project, including review of correlation software and use of confocal microscopy toward certifying a reference standard.

Teaching Experience

- Virginia Tech, Blacksburg, VA
  Graduate Teaching Assistant, Department of Physics
  - Fall 2015 – Spring 2018 Physics Major Tutor and Recitation Lecturer
  - October 2016 Four lectures of PHYS 5714: Graduate Mathematical Methods
  - Spring 2014 PHYS 2305: Foundations of Physics I laboratory
  - Fall 2013 PHYS 2215: General Physics I laboratory

- Appalachian State University, Boone, NC
  Teaching Assistant, Department of Physics and Astronomy
  - Fall 2012 PHY 3010: Classical Mechanics I

  Physics Tutor, University Tutoring Center
  - Fall 2010 – Fall 2011 Analytical Physics (calculus-based)

Computing Experience

- Fortran, C++, MPI (single node, multi-core).
- VASP (Vienna Ab-initio Simulation Package), QE (Quantum Espresso), and SIESTA for DFT calculations, Wannier90, PHONOPY, WannierTools, Mathematica

Publications

Under review:

1. John W. Villanova, Saban Hus, Seoung-Hun Kang, Hoyeon Jeon, An-Ping Li, David Mandrus, Zheng Gai, and Mina Yoon, "Surface structure and ghost state of the charge density wave kagome metal ScV6Sn6." (submitted)

2. Colin L. Sarkis, John W. Villanova, Casey Eichstaedt, Adolfo G. Eguiluz, Jaime A. Fernandez-Baca, Masaaki Matsuda, Jiaqiang Yan, Christian Balz, Arnab Banerjee, D. Alan Tennant, Tom Berlijn, and Stephen E. Nagler, "Experimental Evidence for Non-spherical Form Factor in Ru^{3+}." (**Accepted** for publication in Phys. Rev. B as an **Editor's Suggestion**)

3. Shirin Mozaffari, William R. Meier, Richa P. Madhorgaria, Seoung-Hun Kang, John W. Villanova, Hasitha W. Suriya Arachchige, Guoxin Zheng, Yuan Zhu, Kuan-Wen Chen, Kaila Jenkins, Dechen Zhang, Aaron Chan, Lu Li, Mina Yoon, Yang Zhang, and David G. Mandrus, "Universal sublinear resistivity in vanadium kagome materials hosting charge density waves," arXiv: 2305.02393v1. (submitted)

4. Seoung-Hun Kang, Haoxiang Li, William R. Meier, John W. Villanova, Saban Hus, Hoyeon Jeon, Hasitha W. Suriya Arachchige, Qiangsheng Li, Zheng Gai, Jonathan Denlinger, Rob Moore, Mina Yoon, and David Mandrus, "Emergence of a new band and the Lifshitz transition in kagome metal ScV6Sn6 with charge density wave," arXiv: 2302.14041v1. (submitted)

Published:

1. A. O. Scheie, Y. Kamiya, Hao Zhang, Sangyun Lee, A. J. Woods, M. G. Gonzalez, B. Bernu, John W. Villanova, J. Xing, Q. Huang, Qing Ming Zhang, Jie Ma, Eun Sang Choi, D. M. Pajerowski, Haidong Zhou, A. S. Sefat, S. Okamoto, T. Berlijn, L. Messio, R. Movshovich, C. D. Batista, D. A. Tennant, "Non-linear magnons and exchange Hamiltonians of the delafossite proximate quantum spin liquid candidate KYbSe2 and NaYbSe2," Phys. Rev. B **109**, 014425 (2024). **(Editor's Suggestion)**

2. Randy S. Fishman, Tom Berlijn, Jack Villanova, and Lucas Lindsay, "Magnon orbital angular momentum of ferromagnetic honeycomb and zigzag lattice models," Phys. Rev. B **108**, 214402 (2023).

3. Allen O. Scheie, Pyeongjae Park, John W. Villanova, G. E. Granroth, Colin L. Sarkis, Hao Zhang, M. B. Stone, Je-Geun Park, Satoshi Okamoto, Tom Berlijn, and D. Alan Tennant, "Spin wave Hamiltonian and anomalous scattering in NiPS3," Phys. Rev. B **108**, 104402 (2023). **(Editor's Suggestion)**

4. John W. Villanova, Allen O. Scheie, D. Alan Tennant, Satoshi Okamoto, and Tom Berlijn, "First-principles derivation of magnetic interactions in the triangular quantum

spin liquid candidates $KYbCh_2$ (Ch=S, Se, Te) and $AYbSe_2$ (A=Na,Rb)," Phys. Rev. Research **5**, 033050 (2023).

5. Joseph E. Roll, John M. Davis, John W. Villanova, and Salvador Barraza-Lopez, "Elasticity of two-dimensional ferroelectrics across their paraelectric phase transformation," Phys. Rev. B **105**, 214105 (2022).

6. Krishna Pandey, Debashis Mondal, John W. Villanova, Joseph Roll, Rabindra Basnet, Aaron Wegner, Gokul Acharya, Md Rafique Un Nabi, Barun Ghosh, Jun Fujii, Jian Wang, Bo Da, Amit Agarwal, Ivana Vobornik, Antonio Politano, Salvador Barraza-Lopez, Jin Hu, "Magnetic Topological Semimetal Phase with Electronic Correlation Enhancement in SmSbTe." Adv. Quantum Technol. 4, 2100063 (2021).

7. Kai Chang, John W. Villanova, Jing-Rong Ji, Souvik Das, Felix Küster, Salvador Barraza-Lopez, Paolo Sessi, and Stuart S. P. Parkin, "Vortex-oriented ferroelectric domains in SnTe/PbTe monolayer lateral heterostructures." Adv. Mater. 2102267 (2021).

8. Salvador Barraza-Lopez, Benjamin M. Fregoso, John W. Villanova, Stuart S. P. Parkin, and Kai Chang, "Colloquium: Physical properties of group-IV monochalcogenides monolayers." Rev. Mod. Phys. **93**, 011001 (2021).

9. John W. Villanova and Salvador Barraza-Lopez, "Anomalous thermoelectricity at the two-dimensional structural transition of SnSe monolayers." Phys. Rev. B **103**, 036421 (2021).

10. John W. Villanova, Pradeep Kumar, and Salvador Barraza-Lopez, "Theory of finite-temperature two-dimensional structural transformations in group-IV monochalcogenide monolayers." Phys. Rev. B **101** 184101 (2020).

11. Yichul Choi, John W. Villanova, and Kyungwha Park, "Zeeman-splitting-induced topological nodal structure and anomalous Hall conductivity in ZrTe5." Phys. Rev. B **101** 035105 (2020).

12. Shiva P. Poudel, John W. Villanova, and Salvador Barraza-Lopez, "Group-IV monochalcogenide monolayers: Two-dimensional ferroelectrics with weak intralayer bonds and a phosphorenelike monolayer dissociation energy." Phys. Rev. Materials **3**, 124004 (2019).

13. John W. Villanova and Kyungwha Park, "Magnetic field induced Weyl semimetal from Wannier-function-based tight-binding model." Phys. Rev. B **98** 075123 (2018).

14. John W. Villanova, Edwin Barnes, and Kyungwha Park, "Engineering and Probing Topological Properties of Dirac Semimetal Films by Asymmetric Charge Transfer." Nano Letters **17** (2), 963-972 (2017).

15. John W. Villanova and Kyungwha Park, "Spin Textures of topological surface states at side surfaces of Bi_2Se_3 from first principles." Phys. Rev. B **93** 085122 (2016).

16. Xiaoyu A. Zheng, Johannes A. Soons, Robert M. Thompson, John Villanova, Taher Kakal, "2D and 3D Topography Comparisons of Toolmarks Produced from Consecutively Manufactured Chisels and Punches." AFTE Journal, 46 143-7 (2014).

Presentations at Conferences

1. "Simulating magnetic form factors of Kitaev materials." Poster presentation at the Quantum Science Center All-Hands Meeting, Nashville, TN, May 21-24 (2023). **[*Selected as a Best Poster Award*]**
2. "Simulating magnetic form factors of Kitaev materials." Talk at the American Physical Society March Meeting, Las Vegas, NV, March 6-10 (2023).
3. "Softening phonon modes drive the structural phase transition in silicene." Talk at the (Online) American Physical Society March Meeting, Nashville, TN, March 15-19 (2021).
4. "Thermoelectricity of SnSe monolayers across a structural phase transition." Talk at the (Online) Conference on Transport at the Nanoscale, October 12-16 (2020).
5. "Structural constraints and the spatial electronic distribution determine the transition temperature of two-dimensional ferroelectrics." Talk at the 9th International Conference on Low Dimensional Structures and Devices, Puerto Varas, Chile, December 2-6 (2019).
6. "On the mechanism for the 2D phase transition in freestanding group-IV monochalcogenide monolayers." Talk at the American Physical Society March Meeting, Boston, MA, March 4-8 (2019)
7. "Evolution of Fermi-arc surface states in a magnetic-field induced Weyl semimetal." Talk at the American Physical Society March Meeting, Los Angeles, CA, March 5-9 (2018)
8. "Engineering and probing topological properties of Dirac semimetal films by asymmetric charge transfer." Poster presentation at the Electronic Structure Workshop 2017, Princeton, NJ, June 25-28 (2017)
9. "Topological Dirac semimetal Na_3Bi: substrate and B-field effects." Poster presentation at the CREST IDEALS Community Meeting, CCNY, New York City, NY, April 21 (2017)
10. "Engineering and probing topological properties of Dirac semimetal films by asymmetric charge transfer." Talk at the American Physical Society March Meeting, New Orleans, LA, March 13-17 (2017)
11. "Spin texture of topological surface states on the side-surfaces of Bi_2Se_3." Poster presentation at the Electronic Structure Workshop 2016, Albuquerque, NM, June 26-29 (2016)

12. "Spin textures of topological surface states at side surfaces of Bi_2Se_3 from first principles." Talk at the American Physical Society March Meeting, Baltimore, MD, March 14-18 (2016).

Service

- Graduate Student Representative to the Graduate Committee, Virginia Tech, Fall 2016 – Summer 2017

Honors and Awards

- Quantum Science Center All-Hands Meeting Best Poster Award, May 2023
- CREST IDEALS (interface design and engineered assembly of low-dimensional systems) Fellowship from CCNY, January 2017 - August 2018
- William E. Hassinger Graduate Fellowship, Fall 2016
- Graduate School Doctoral Assistantship, Spring 2016
- Phillip Morris Physics Fellowship, Fall 2013
- Walter C. Connolly Award, Spring 2013

Affiliations

- The American Physical Society