# **Liangbo Liang**

Senior Research & Development Staff Center for Nanophase Materials Sciences (CNMS) Oak Ridge National Laboratory (ORNL) (865) 576-5134 <u>liangl1@ornl.gov</u> <u>Publications</u>

## Education

Rensselaer Polytechnic Institute (RPI), U.S.A. Wuhan University, China Physics Physics

Ph.D., 2014 B.S., 2008

## **Research Areas**

## Theoretical Condensed Matter Physics; Computational Physics; First-principles Density Functional Theory; Many-body GW Method; Quantum Materials; Nanomaterials

- 1. Theoretical research on diverse properties of quantum materials and nanomaterials, including their electronic, magnetic, optical, vibrational, thermal, thermoelectric, piezoelectric, photovoltaic properties, etc.
- 2. Developing and applying computational packages for quantum modeling of various experimental techniques, such as scanning tunneling microscopy/spectroscopy, Raman spectroscopy, photoluminescence spectroscopy, etc.
- 3. Close collaborations with experimentalists across the world to explain and guide experimental measurements on diverse systems ranging from molecules to nanomaterials to strongly correlated materials.

## **Research Projects**

CNMS Theme Science: "Heterogeneities in Quantum Materials".

**CNMS In-house Research:** "Integration of Accurate Theoretical/Computational Approaches with Experimental Techniques for the Understanding of Quantum Materials and Nanomaterials".

#### **Professional Experience**

Senior Research Staff, Center for Nanophase Materials Sciences, ORNL2025–PresenResearch Staff, Center for Nanophase Materials Sciences, ORNL2018–2025	
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Eugene Wigner Fellow/Research Staff Associate, Center for Nanophase Materials Sciences, ORNL 2015–2018	
Postdoctoral Research Associate, Department of Physics, RPI (Supervisor: Dr. Vincent Meunier) 2014–2015	5
Graduate Research Assistant, Department of Physics, RPI (Advisor: Dr. Vincent Meunier) 2010–2014	1
Professional and Synergistic Activities	
Member and the Treasurer of the Executive Committee of the APS Mid-Atlantic Section 2023–Presen	t
Co-organizer of 2024 Annual Meeting of the APS Mid-Atlantic Section 2024	
Invited Talk at 2024 CNMS User Meeting Quantum Workshop 2024	
Early Career Editorial Board Member with Journal "Carbon Trends" of Elsevier 2023–Presen	
Co-organizer of 2023 Annual Meeting of the APS Mid-Atlantic Section 2023	
Organized 2023 CNMS User Meeting Workshop "Novel Materials for Neuromorphic Computing" 2023	
Invited Talk at the 8th NANO Boston Conference 2022	
Invited Talk at the 7th NANO Boston Conference 2021	
Invited Talk at the 3rd International Conference on Advances in Functional Materials (AAAFM-UCLA) 2021	
Invited Talk at the seminar series "Theory Talks" at Lawrence Berkeley National Laboratory 2021	
Invited Talk at the GrapheneforUS 2019 International Conference 2019	
Invited Talk at 2019 CNMS User Meeting 2019	
Invited Talk at the Fifth Wuhan University International Forum (China) 2018	
Invited Talk at Graphene Week 2017 (Greece) 2017	
Invited Talk at 2017 CNMS-SNS User Meeting Workshop 2017	7
Program Coordinator for International Phosphorene Symposium 2015	5
Referee to journals: Nature, Nature Nanotechnology, Nature Materials, Nature Communications, ACS Nano, Nano Letters, Physical Review Letters, Nanoscale, Carbon, Scientific Reports, Small, Nanotechnology, 2D Materials, etc.	

Reviewer for proposals: DOE, ORNL LDRD, ORNL/UTK JDRD, NSF CAREER

#### **Honors and Awards**

ORNL Supplemental Performance Award CNMS Division Award: Most Notable CNMS User Project 2025 2023

UT-Battelle/ORNL Award: Outstanding Scholarly Output Team Award	2020
CNMS Division Award: Distinguished Scientific Paper	2017
CNMS Division Award: Outstanding Scientific or Technical Contribution	2017
CNMS Division Award: Most Notable CNMS User Project	2016
Eugene Wigner Fellowship of Oak Ridge National Laboratory	2015
Outstanding Reviewer - Journal Carbon	2015
Hillard Huntington Award for Outstanding Graduate Student (for top one of the Department at RPI)	2014
First Prize of the National Scholarship (for top one of the class at Wuhan University)	2007
Samsung Scholarship (for top one of the Department at Wuhan University)	2006

#### **Selected Publications**

(120+ publications in total with 14,000+ citations, h-index=48 from Google Scholar/43 from Web of Science, including papers in high-impact journals such as Nature Nanotechnology, Nature Communications, Science Advances, Physical Review Letters, Nano Letters, ACS Nano, JACS, Advanced Materials, PNAS, Nanoscale, Angewandte Chemie, npj 2D Materials, etc.)

- 1. X. Kong, P. Ganesh, L. Liang\*, "First-principles study of the magneto-Raman effect in van der Waals layered magnets", *npj 2D Materials and Applications*, 8, 82 (2024). [\*Corresponding author]
- S. Yang, L. Liang\*, Y. Lee, Y. Gu, J. Fatheema, S. Kutagulla, D. Kim, M. Kim, S. Kim, D. Akinwande, "Volatile and Nonvolatile Resistive Switching Coexistence in Conductive Point Hexagonal Boron Nitride Monolayer", ACS Nano, 18, 4, 3313–3322 (2024). [\*Co-lead author]
- Y. Pai, C. Marvinney, G. Pokharel, J. Xing, H. Li, X. Li, M. Chilcote, M. Brahlek, L. Lindsay, H. Miao, A. Sefat, D. Parker, S. Wilson, J. Gardner, L. Liang\*, B. Lawrie, "Angular-Momentum Transfer Mediated by a Vibronic-Bound-State", *Advanced Science*, 2304698 (2023). [\**Corresponding author*]
- X. Kong, W. Luo, L. Li, M. Yoon, T. Berlijn, L. Liang\*, "Floquet band engineering and topological phase transition in 1T' transition metal Dichalcogenides", 2D Materials, 9, 025005 (2022). [\*Corresponding author]
- P. Joshi, R. Li, J. Spellberg, L. Liang\*, S. King\*, "Nanoimaging of the Edge-Dependent Optical Polarization Anisotropy of Black Phosphorus", *Nano Letters*, 22, 8, 3180 (2022). [\**Co-corresponding author*]
- X. Wang, J. Cao, H. Li, Z. Lu, A. Cohen, A. Haldar, H. Kitadai, Q. Tan, K. Burch, D. Smirnov, W. Xu, S. Sharifzadeh, L. Liang, X. Ling, "Electronic Raman scattering in the 2D antiferromagnet NiPS<sub>3</sub>", *Science Advances*, 8 (2), eabl7707 (2022).
- 7. X. Kong, T. Berlijn, L. Liang\*, "Thickness and spin dependence of Raman modes in magnetic layered Fe<sub>3</sub>GeTe<sub>2</sub>", *Advanced Electronic Materials*, 2001159 (2021). [\**Corresponding author*]
- 8. X. Kong, H. Yoon, M. J. Han, L. Liang<sup>\*</sup>, "Switching interlayer magnetic order in bilayer CrI<sub>3</sub> by stacking reversal", *Nanoscale*, 13, 16172 (2021). [\**Corresponding author*]
- R. Ge\*, X. Wu\*, L. Liang\*, S. Hus, Y. Gu, E. Okogbue, H. Chou, J. Shi, Y. Zhang, S. Banerjee, Y. Jung, J. Lee, D. Akinwande, "A Library of Atomically Thin 2D Materials Featuring the Conductive-Point Resistive Switching Phenomenon", *Advanced Materials*, 33, 2007792 (2021). [\**Co-lead author*]
- S. Hus, R. Ge, P. Chen, L. Liang, G. Donnelly, W. Ko, F. Huang, M. Chiang, A. Li, D. Akinwande, "Observation of single-defect memristor in an MoS<sub>2</sub> atomic sheet", *Nature Nanotechnology*, 16, 58–62 (2021).
- 11. W. Luo, A. Oyedele, Y. Gu, T. Li, X. Wang, A. Haglund, D. Mandrus, A. Puretzky, K. Xiao, L. Liang\*, X. Ling\*, "Anisotropic Phonon Response of Few-Layer PdSe<sub>2</sub> under Uniaxial Strain", *Advanced Functional Materials*, 2003215 (2020). [\**Co-corresponding author*]
- G. Nguyen, A. Oyedele, A. Haglund, W. Ko, L. Liang\*, A. Puretzky, D. Mandrus, K. Xiao, A. Li\*, "Atomically Precise PdSe<sub>2</sub> Pentagonal Nanoribbons", ACS Nano, 14, 1951 (2020). [\*Co-corresponding author]
- J. Zhang, X. Li, K. Xiao, B. Sumpter, A. Ghosh, L. Liang\*, "The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides", *Journal of Physics: Condensed Matter*, 32, 025306 (2019). [\**Corresponding author*]
- L. Liang, E. C. Girão, V. Meunier, "Modeling the Kondo effect of a magnetic atom adsorbed on graphene", 2D Materials, 6, 035038 (2019).
- N. Mao, X. Wang, Y. Lin, B. Sumpter, Q. Ji, T. Palacios, S. Huang, V. Meunier, M. Dresselhaus, W. Tisdale, L. Liang\*, X. Ling\*, J. Kong\*, "Direct Observation of Symmetry-Dependent Electron-Phonon Coupling in Black Phosphorus", *Journal of the American Chemical Society*, 141, 18994 (2019). [\**Co-corresponding author*]
- W. Zhu\*, L. Liang\*, R. Roberts, J. Lin, D. Akinwande, "Anisotropic Electron–Phonon Interactions in Angle-Resolved Raman Study of Strained Black Phosphorus", ACS Nano, 12, 12512 (2018). [\*Co-lead author]

- A. Puretzky, A. Oyedele, K. Xiao, A. V. Haglund, B. Sumpter, D. Mandrus, D. B. Geohegan, L. Liang\*, "Anomalous interlayer vibrations in strongly coupled layered PdSe<sub>2</sub>", *2D Materials*, 5, 035016 (2018). [\**Corresponding author*]
- G. D. Nguyen, L. Liang\*, Q. Zou, M. Fu, A. Oyedele, B. Sumpter, Z. Liu, Z. Gai, K. Xiao, A. Li\*, "3D imaging and manipulation of subsurface selenium vacancies in PdSe<sub>2</sub>", *Physical Review Letters*, 121, 086101 (2018). [\**Co-corresponding author*]
- L. Liang\*, A. Puretzky, B. Sumpter, V. Meunier, "Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials", *Nanoscale*, 9, 15340 (2017). [\**Corresponding author*]
- L. Liang, J. Zhang, B. Sumpter, Q. Tan, P. Tan, V. Meunier, "Low-Frequency Shear and Layer-Breathing Modes in Raman Scattering of Two-Dimensional Materials", ACS Nano, 11, 11777 (2017).
- C. Ma, L. Liang\*, Z. Xiao, A. Puretzky, W. Lu, V. Meunier, J. Bernholc, A. Li\*, "Seamless staircase electrical contact to semiconducting graphene nanoribbon", *Nano Letters*, 17, 6241 (2017). [\**Co-corresponding author*]
- 22. L. Liang, V. Meunier, "Atomically Precise Graphene Nanoribbon Heterojunctions for Excitonic Solar Cells", *The Journal of Physical Chemistry C*, 119, 775 (2015).
- 23. L. Liang, J. Wang, W. Lin, B. G. Sumpter, V. Meunier, M. Pan, "Electronic Bandgap and Edge Reconstruction in Phosphorene Materials", *Nano Letters*, 14, 6400 (2014).
- L. Liang, V. Meunier, "First-principles Raman spectra of MoS<sub>2</sub>, WS<sub>2</sub> and their heterostructures", *Nanoscale*, 6, 5394 (2014).
- 25. L. Liang, E. Cruz-Silva, E. C. Girão, V. Meunier, "Enhanced thermoelectric figure of merit in assembled graphene nanoribbons", *Physical Review B*, 86, 115438 (2012).

#### **Teaching and Mentoring Experience**

Mentoring Postdocs, Oak Ridge National Laboratory	2019-Present
(e.g., Xiangru Kong, now assistant professor at Northeastern University, China)	
Co-mentoring Students, Oak Ridge National Laboratory	2015-Present
(e.g., Natalya Sheremetyeva and Andrew Cupo, Rensselaer Polytechnic Institute; Jingjie Zhang,	University of
Virginia; Weijun Luo, Boston University; Jameela Fatheema, University of Texas at Austin)	
Serving on the dissertation committee of PhD and Master students	2017-Present
(Weijun Luo, Boston University; Jameela Fatheema, University of Texas at Austin; Sung Jin Yang,	University of
Texas at Austin; João Fernandes, University of Minho)	
Mentoring Students and Postdoctoral Researchers, Department of Physics, RPI	2013-2015
(e.g., Pan Zhu and Daniel Massote, Rensselaer Polytechnic Institute)	
Graduate Teaching Assistant, Department of Physics, RPI	2010-2012