

# Liangbo Liang

Research & Development Staff  
Center for Nanophase Materials Sciences (CNMS)  
Oak Ridge National Laboratory (ORNL)  
(865) 576-5134  
[liangl1@ornl.gov](mailto:liangl1@ornl.gov)  
[Publications](#)



---

## Education

Rensselaer Polytechnic Institute (RPI), U.S.A.	Physics	Ph.D., 2014
Wuhan University, China	Physics	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

Research Staff, Center for Nanophase Materials Sciences, ORNL	2018–Present
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
Graduate Research Assistant, Department of Physics, RPI (Advisor: Dr. Vincent Meunier)	2010–2014

## Professional and Synergistic Activities

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
Program Coordinator for International Phosphorene Symposium	2015
Invited Talk at the Physics Colloquium at Rensselaer Polytechnic Institute	2013

Referee to journals: Nature, Nature Nanotechnology, Nature Materials, Nature Communications, ACS Nano, Nanoscale, Carbon, Scientific Reports, Small, Nanotechnology, 2D Materials, Journal of Raman Spectroscopy, etc.

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

## Honors and Awards

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

(100+ publications in total with 9,200+ citations, h-index=42 from Google Scholar/40 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, 2D Materials, etc.)

1. X. Kong, T. Berlijn, **L. Liang\***, “Thickness and spin dependence of Raman modes in magnetic layered  $\text{Fe}_3\text{GeTe}_2$ ”, *Advanced Electronic Materials*, 2001159 (2021). [\*Corresponding author]
2. X. Kong, H. Yoon, M. J. Han, **L. Liang\***, “Switching interlayer magnetic order in bilayer  $\text{CrI}_3$  by stacking reversal”, *Nanoscale*, 13, 16172 (2021). [\*Corresponding author]
3. 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]
4. 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  $\text{MoS}_2$  atomic sheet”, *Nature Nanotechnology*, 16, 58–62 (2021).
5. W. Luo, A. Oyedele, Y. Gu, T. Li, X. Wang, A. Haglund, D. Mandrus, A. Puretzy, K. Xiao, **L. Liang\***, X. Ling\*, “Anisotropic Phonon Response of Few-Layer  $\text{PdSe}_2$  under Uniaxial Strain”, *Advanced Functional Materials*, 2003215 (2020). [\*Co-corresponding author]
6. G. Nguyen, A. Oyedele, A. Haglund, W. Ko, **L. Liang\***, A. Puretzy, D. Mandrus, K. Xiao, A. Li\*, “Atomically Precise  $\text{PdSe}_2$  Pentagonal Nanoribbons”, *ACS Nano*, 14, 1951 (2020). [\*Co-corresponding author]
7. 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]
8. **L. Liang**, E. C. Girão, V. Meunier, “Modeling the Kondo effect of a magnetic atom adsorbed on graphene”, *2D Materials*, 6, 035038 (2019).
9. 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]
10. 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]
11. A. Puretzy, A. Oyedele, K. Xiao, A. V. Haglund, B. Sumpter, D. Mandrus, D. B. Geohegan, **L. Liang\***, “Anomalous interlayer vibrations in strongly coupled layered  $\text{PdSe}_2$ ”, *2D Materials*, 5, 035016 (2018). [\*Corresponding author]
12. 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  $\text{PdSe}_2$ ”, *Physical Review Letters*, 121, 086101 (2018). [\*Co-corresponding author]
13. **L. Liang\***, A. Puretzy, B. Sumpter, V. Meunier, “Interlayer bond polarizability model for stacking-dependent low-frequency Raman scattering in layered materials”, *Nanoscale*, 9, 15340 (2017). [\*Corresponding author]
14. **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).
15. C. Ma, **L. Liang\***, Z. Xiao, A. Puretzy, W. Lu, V. Meunier, J. Bernholc, A. Li\*, “Seamless staircase electrical contact to semiconducting graphene nanoribbon”, *Nano Letters*, 17, 6241 (2017). [\*Co-corresponding author]
16. **L. Liang**, V. Meunier, “Atomically Precise Graphene Nanoribbon Heterojunctions for Excitonic Solar Cells”, *The Journal of Physical Chemistry C*, 119, 775 (2015).
17. **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).
18. **L. Liang**, V. Meunier, “First-principles Raman spectra of  $\text{MoS}_2$ ,  $\text{WS}_2$  and their heterostructures”, *Nanoscale*, 6, 5394 (2014).
19. **L. Liang**, V. Meunier, “Electronic and thermoelectric properties of assembled graphene nanoribbons with elastic strain and structural dislocation”, *Applied Physics Letters*, 102, 143101 (2013).
20. **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/Co-advising Students, Oak Ridge National Laboratory (e.g., Natalya Sheremetyeva and Andrew Cupo, Rensselaer Polytechnic Institute; Jingjie Zhang, University of Virginia; Weijun Luo, Boston University)	2015-Present
Mentoring Students and Postdoctoral Researchers, Department of Physics, RPI (e.g., Pan Zhu and Daniel Massote, Rensselaer Polytechnic Institute)	2013-2015
Graduate Teaching Assistant, Department of Physics, RPI	2010-2012