A person wearing a suit and tie

Description automatically generated**Kai Xiao, Ph.D.**

Distinguished R&D Staff Scientist and UT/ORNL Joint Faculty

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[**Website**](https://kaixiao.ornl.gov/)**:** **http://kaixiao.ornl.gov**

[**Google Scholar**](https://scholar.google.com/citations?user=s1J22jMAAAAJ&hl=en)

**Education:**

Ph.D. (2004), *Physical Chemistry,* Institute of Chemistry, Chinese Academy of Sciences, Beijing, China

M.S. (2001), *Materials Science,* Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China

B.S. (1998), *Chemistry,* East China Institute of Technology, China

**Research Expertise:**

* ~ 20 Years Research Experience in synthesis, characterization, and devices of functional nanomaterials and thin films.
* Expertise in the development of advanced manufacturing methods including CVD, PLD, printing, and solution-processing approaches, for growing functional nanomaterials and thin films for microelectronics, quantum information and energy-related applications.
* Expertise in the utilization of in situ characterizations to understand the structure evolution during the synthesis and processing, growth mechanism and kinetics, and functionality by x-ray diffraction, neutron scattering/reflectivity, TEM/STEM, and optical spectroscopies.
* Expertise in the fabrication of nanoelectronic devices (FET, photodetectors, etc) by e-beam lithography and photolithography and characterization of devices to understand the optoelectronic and quantum properties.
* Expertise in the fabrication and characterization of solution-processing thin film electronic devices (FET, photodetector, photovoltaic) for energy conversion and flexible electronics.
* Functional nanomaterials: 2D quantum materials, halide perovskites, conducting polymers.

**Research and Professional Experience:**

2023-present Distinguished Staff Scientist, CNMS, ORNL

2018- *2023* Senior R&D Staff Scientist, CNMS, ORNL

* Understanding the fundamental growth mechanism and kinetics of 2D quantum materials and heterostructures for microelectronics, quantum information science and energy-related applications. Serving as PI on a BES-MSED FWP “Growth Mechanisms and Controlled Synthesis of Nanomaterials” that focuses on understanding the synthesis and processing of 2D materials such as the transition metal dichalcogenides and moiré heterostructures by the development of practical, time-resolved in situ diagnostic techniques for characterization of both the growth environment and the evolving 2D quantum structure during pulsed processing, focusing on PLD and laser processing as versatile non-equilibrium synthesis and processing tools over three length scales with closed loop control. The goal of this project is to identify and understand the dynamic pathways and interactions leading to the assembly of functional quantum nanostructures.
* Developed a 2D materials transfer station in glove box for exfoliate, transfer, and encapsulation of air-sensitive 2D quantum materials to make moiré materials and heterostructures.

2011- *Present* Joint faculty in Department of Computer Science and Electrical Engineering and the Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee Knoxville

2013-*2017* R&D Staff Scientist, CNMS, ORNL

* Controlled synthesis and characterization of hybrid perovskites by solution processing and spray printing with various in situ diagnostic methods at multiple length scales including XRD, neutron scattering, and TEM for high efficiency solar cells.
* Tailored the heterogeneity in 2D materials and heterostructures through controlled CVD synthesis and processing for high performance transistors, photodetectors and photovoltaics

2008-2013 R&D Associate, CNMS, ORNL

* Developed a strategy to understand and control the morphology, structure and correlated optoelectronic properties of conducting block copolymers and their composites by advanced electron microscopy, neutron scattering/reflectivity and theoretical modeling for high performance electronics and organic photovoltaics.

2004-2008 Postdoctoral Associate, *CNMS, ORNL* (Mentor: David B Geohegan)

* Initially worked on CVD synthesis and selective patterning of organic semiconductor nanowires and their applications in field effect transistor and flexible non-volatile memory devices. The vapor-solid chemical reaction (VSCR) growth mechanism was revealed by time-resolved, in situ X-ray diffraction (XRD) and first-principles atomistic calculations.
* Developed the hybrid materials assembly facility at CNMS for synthesis, assembly, and device fabrication of air-sensitive, solution-processible materials for organic thin film electronics and flexible electronics, including OFET, OLED, and OPVs.

**Fundings:**

2021- 2024DOE Office of Science, BES Materials Science and Engineering Division. “Growth Mechanisms and Controlled Synthesis of Nanomaterials”. (Kai Xiao, PI)

2015- 2020DOE Office of Science, BES Materials Science and Engineering Division. “Growth Mechanisms and Controlled Synthesis of Nanomaterials”. (David Geohegan, PI) (Xiao, Co-PI)

2018- 2021 DOE Office of Science, BES, Quantum Information Science NSRC “Thin Film Platform for Rapid Prototyping of Novel Materials with Entangled States for QIS.” (Chris Rouleau, PI), (Xiao, Co-PI)

2018-2019 ORNL LDRD “Interfacial Thermal Transport: Advanced First Principles Modeling and Ultrafast Thermal Spectroscopy”. (Lucas Lindsay, PI, Xiao, Co-PI)

2015-2017 ORNL LDRD: “Synthesis and Characterization of Novel Two-Dimensional Mesoscale Organic Nanomembranes.” (Xiao, PI).

2012-2014 DOE-EERE “Novel photon management for thin-film photovoltaics” (Rajesh Menon, University of Utah PI), (Xiao, Co-PI)

2009-2011 ORNL LDRD “Rational design of deuterated conjugated polymers with controlled spin-polarized electron transport.” (Keum, PI), (Xiao, co-PI).

**Invited Book Chapters:**

1. D. B. Geohegan, K. Xiao, A.A. Puretzky, Y.-C. Lin, Y. Yu, C. Liu, Nonequilibrium synthesis and processing approaches to tailor heterogeneity in 2D Materials, Chapter 8, in Defects in Two-Dimensional Materials, Elsevier, pp 221-458 (2022).
2. B. Yang, MJ. Keum, D. B. Geohegan and K. Xiao, “In Situ X-Ray Studies of Crystallization Kinetics and Ordering in Functional Organic and Hybrid Materials”, Chapter 2 in In-situ Characterization Techniques for Nanomaterials, Spring Series on Nanoscience and Nanotechnology, Vol. 7, 2018, pp 33-60.
3. B. Yang, D. B. Geoghegan, K. Xiao, "Perovskite Materials: Solar Cells and Optoelectronic Applications" in Encyclopedia of Inorganic and Bioinorganic Chemistry, ed R. A. Scott, John Wiely: Chichester. DOI: 10.1002/9781119951438. Published 15 March 2017.
4. B. Yang, M. Shao, J. Keum, D. B. Geohegan and K. Xiao, "Nanophase Engineering of Organic Semiconductor-Based Solar Cells", Chapter 7 in Semiconductor Materials for Solar Photovoltaic Cells, Springer Series in Materials Science, Vol 218, 2015, pp 197-229.
5. D. B. Geohegan, A. A. Puretzky, M. Yoon, G. Eres, C. Rouleau, K. Xiao, J. Jackson, J. Readle, M. Regmi, N. Thonnard, G. Duscher, M. Chisholm and K. More, "Laser Interactions for the Synthesis and In Situ Diagnostics of Nanomaterials", Chapter 7 in Lasers in Materials Science, Springer Series in Materials Science, Vol 191, 2014, pp 143-173.
6. D. B. Geohegan, A. A. Puretzky, C. M. Rouleau, J. J. Jackson, G. Eres, Z. Liu, D. Styers-Barnett, H. Hu, B. Zhao, K. Xiao, I. Ivanov, and K. More, "Laser Interactions in Nanomaterials Synthesis," Chapter 1 in Laser-Surface Interactions for New Materials Production: Tailoring Structure and Properties, Springer Series in Materials Science, Vol. 130, Miotello, Antonio; Ossi, Paolo M., Eds. ISBN: 978-3-642-03306-3 (2010).
7. X. B. Sun, K. Xiao, D. Q. Zhang, Y. Q. Liu, D. B. Zhu, "Organic Semiconductor Materials," Chapter in Materials Science and Engineering, Eds. C. X. Shi, H. D. Li, and L. Zhou, Chemical Engineering Publishers, Beijing, China (2004).

**Journal Articles Published in Peer Reviewed Journals: [Total:>180; Citations:> 14900; h-index: 66 on google scholar]**

Selected 20 publications (followed by a complete list of publications)

1. K. Xiao\*, D. B. Geohegan\*, Laser synthesis and processing of atomically thin 2D materials, Trends in Chemistry, 4, 769(2022).
2. Y. Gu, L. Zhang, H. Cai, L. Liang, C. Liu, A. Hoffman, Y. Yu, A. Houston, A. A. Puretzky, G. Duscher, P. D. Rack, C. M. Rouleau, X. Meng, M. Yoon, D. B. Geohegan, K. Xiao\*, Stabilized synthesis of 2D verbeekite: Monoclinic PdSe2 crystals with high mobility and in-plane optical and electrical anisotropy, ACS Nano. 16, 13900 (2022). **Note: This work was highlighted as the journal cover.**
3. K. Wang, L. Zhang, G. D Nguyen, X. Sang, C. Liu, Y. Yu, W. Ko, R. R Unocic, A. A Puretzky, C. M Rouleau, D. B Geohegan,. Fu, G. Duscher, A.‐P. Li, M. Yoon, K. Xiao\*, Selective Antisite Defect Formation in WS2 Monolayers via Reactive Growth on Dilute W‐Au Alloy Substrates, Advanced Materials, 34(3), 2106674(2022). **Note: This work was highlighted as the journal Frontpieces.**
4. H. Cai, Y. Yu, Y.-C. Lin, A. A. Puretzky, D. B. Geohegan, K. Xiao\*, “Heterogeneities at multiple length scales in 2D layered materials: From localized defects and dopants to mesoscopic heterostructures”, Nano Research, 14, 1625 (2021). **Invited Review and Back cover.**
5. Y. Gu, H. Cai, J. Dong, Y. Yu, A. N Hoffman, C. Liu, A. D Oyedele, Y‐C. Lin, Z. Ge, A. A Puretzky, G. Duscher, M. F Chisholm, P. D Rack, C. M Rouleau, Z. Gai, X. Meng, F. Ding, D. B Geohegan, K. Xiao\*, “Two‐Dimensional Palladium Diselenide with Strong In‐Plane Optical Anisotropy and High Mobility Grown by Chemical Vapor Deposition”, Advanced Materials 32(19), 1906238 (2020). **Note: This work was selected as the journal cover.**
6. A. Oyedele, S. Yang, T. Feng, A. Haglund, Y. Gu, A. Puretzky, D. Briggs, C. Rouleau, M. Chisholm, R. Unocic, D. Mandrus, S. Pantelides, D. Geohegan, K. Xiao\*, “Defect-Mediated Phase Transformation in Anisotropic Two-Dimensional PdSe2 Crystals for Seamless Electrical Contacts”, J. Am. Chem. Soc. 141, 8928-8936 (2019).
7. K. Wang, A. A Puretzky, Z. Hu, B. R Srijanto, X. Li, N. Gupta, H. Yu, M. Tian, M. Mahjouri-Samani, X. Gao, A. Oyedele, C. Rouleau, G. Eres, B. Yakobson, M. Yoon, K. Xiao\*, D. B Geohegan\*, “Strain tolerance of two-dimensional crystal growth on curved surfaces”, Science Advances 5, eaav4028 (2019). **Note: DOE Office of Science Highlight** [**https://www.energy.gov/science/bes/articles/stretched-limit-and-sparkling-curved-surfaces**](https://www.energy.gov/science/bes/articles/stretched-limit-and-sparkling-curved-surfaces)
8. X. Li, J. Zhang, A. A Puretzky, A. Yoshimura, X. Sang, Q. Cui, Y. Li, L. Liang, A. W Ghosh, H. Zhao, R. R Unocic, V. Meunier, C. M Rouleau, B. G Sumpter, D. B Geohegan, K. Xiao\*, “Isotope-Engineering the Thermal Conductivity of Two-Dimensional MoS2”, ACS Nano 13, 24812 (2019).
9. X. Sang, X. Li, W. Zhao, J. Dong, C. M. Rouleau, D. B. Geohegan, F. Ding, K. Xiao\*, R. R. Unocic, “In situ edge engineering in two-dimensional transition metal dichalcogenides”, Nature Comm, 9, 2051 (2018).
10. B. Yang, W. Ming, M.-H. Du, J. K Keum, A. A Puretzky, C. M Rouleau, J. Huang, D. B Geohegan, X. Wang, K. Xiao\*, “Real-Time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites”, Advanced Materials, 30, 1705801 (2018). **Note: This work was selected as the journal cover.**
11. X. Li, A. A. Puretzky, X. Sang, S. KC, M. Tian, F. Ceballos, M. Mahjouri-Samani, K. Wang, R. R. Unocic, H. Zhao, G. Duscher, V. R. Cooper, C. M. Rouleau, D. B. Geohegan, K. Xiao\*, “Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe2“, Advanced Functional Materials, 27, 1603850 (2017).
12. A. Oyedele, S. Yang, L. Liang, A. Puretzky, K. Wang, J. Zhang, P. Yu, P. Pudasaini, A. Ghosh, Z. Liu, C. Rouleau, B. Sumpter, M. Chisholm, W. Zhou, P. Rack, D. B. Geoghegan, K. Xiao\*, ”PdSe2: Pentagonal 2D Layers with High Air Stability for Electronics” J. Am. Chem. Soc. 139, 14090 (2017). **Note: DOE Office of Science Highlight https://science.osti.gov/bes/Highlights/2018/BES-2018-02-n**
13. X. Li, M.-W. Lin, L. Basile, S. M. Hus, A. A. Puretzky, J. Lee, Y.-C. Kuo, L.-Y. Chang, K. Wang, J. C. Idrobo, A.-P. Li, C.-H. Chen, C. M. Rouleau, D. B. Geohegan, K. Xiao\*, “Isoelectronic tungsten doping in monolayer MoSe2 for carrier type modulation”, Adv Mater, 28, 8240 (2016).
14. X. Li, M.-W. Lin, J. Lin, B. Huang, A. A. Puretzkya, C. Ma, K. Wang, W. Zhou, S. T. Pantelides, C. Miao, I. Kravchenko, J. Fowlkes, C. M. Rouleaua, D. B. Geohegan, K. Xiao\*, “Two- dimensional GaSe/MoSe2 misfit bilayer heterojunctions by van der Waals epitaxy”, Science Advances, 2, E1501882 (2016). **Note: This work has been highlighted by**[***MRS Bulletin***](http://www.google.com/url?q=http%3A%2F%2Fjournals.cambridge.org%2Fdownload.php%3Ffile%3D%252FMRS%252FMRS41_07%252FS0883769416001445a.pdf%26code%3D72410e38b3b79e7f13924f0d065b8fde&sa=D&sntz=1&usg=AFQjCNHwBbZzzypep58jDhscNo-Jv72AxQ)**,**[***Photonics Spectra***](http://www.google.com/url?q=http%3A%2F%2Fwww.photonicsspectra-digital.com%2Fphotonicsspectra%2Fjune_2016%3Fpg%3D24%23pg24&sa=D&sntz=1&usg=AFQjCNENE2TkZrI0aOWUdC0EUqQdDCQNkw)**,**[***ORNL Press***](https://www.google.com/url?q=https%3A%2F%2Fwww.ornl.gov%2Fnews%2Fodd-couple-monolayer-semiconductors-align-advance-optoelectronics&sa=D&sntz=1&usg=AFQjCNE4zwYlICYOiqcwPKBXxcKikwMwrw)**, *Office of Science of DOE*,**[**ScienceDaily**](https://www.google.com/url?q=https%3A%2F%2Fwww.sciencedaily.com%2Freleases%2F2016%2F04%2F160415143756.htm&sa=D&sntz=1&usg=AFQjCNH3cN1qZgxeLRScdmDgdztTBR13GQ)**,**[**Phys.Org**](http://www.google.com/url?q=http%3A%2F%2Fphys.org%2Fnews%2F2016-04-odd-couple-monolayer-semiconductors-align.html&sa=D&sntz=1&usg=AFQjCNGtLvZSAgdHu14vY26_OSgTkFHu-g)**,**[***Optics and Photonics News***](http://www.google.com/url?q=http%3A%2F%2Fwww.osa-opn.org%2Fhome%2Fnewsroom%2F2016%2Fapril%2Fpairing_up_an_optoelectronic_mismatch%2F&sa=D&sntz=1&usg=AFQjCNGuYjakUP6g27BjioO8Y32THav5WQ)**,**[***AAAS EurekAlert***](http://www.google.com/url?q=http%3A%2F%2Fwww.eurekalert.org%2Fpub_releases%2F2016-04%2Fdrnl-cm041416.php&sa=D&sntz=1&usg=AFQjCNE-PQHWYBa9k6ParTbq6DDWNO3ZQg)**, et al.**
15. B. Yang, J. Keum, O. S. Ovchinnikova, A. Belianinov, S. Chen, M.-H. Du, I.N. Ivanov, C.M. Rouleau, D. B. Geohegan, K. Xiao\*, “Deciphering Halogen Competition in Organometallic Halide Perovskite Growth”. J. Am. Chem. Soc. 138, 5028 (2016).
16. B. Yang, O. Dyck, J. Poplawsky, J. Keum, A. Puretzky, S. Das, I. Ivanov, C. Rouleau, G. Duscher, D. Geohegan, and K. Xiao\*, "Perovskite Solar Cells with Near 100% Internal Quantum Efficiency Based on Large Single Crystalline Grains and Vertical Bulk Hetero-junctions", J. Am. Chem. Soc., 137, 9210 (2015). **Note: The work was selected as a Science Highlight by Office of Sciences, U.S. Department of Energy, featured on DOE’s official website “**[**Problem Turned Into Performance for Solar Cells**](https://www.newswise.com/doescience/problem-turned-into-performance-for-solar-cells/?article_id=651138)**”, and released as a Research Highlight in August 2015 CNMS User Newsletter.**
17. M. Shao, J. Keum, J. Chen, Y. He, W. Chen, J. F. Browning, J. Jakowski, B. G. Sumpter, I. N. Ivanov, Y. Ma, C. M. Rouleau,4S. C. Smith, D. B. Geohegan, K. Hong, K. Xiao,\* "The isotopic effects of deuteration on the optoelectronic properties of conducting polymers", Nature Comm. 5, 4180 (2014). **Note: The work was selected as a Science Highlight by Office of Sciences, U.S. Department of Energy, featured on DOE’s official website, and released as a Research Highlight by**[**Materials Views**](http://www.google.com/url?q=http%3A%2F%2Fwww.materialsviews.com%2Fdeuterium-changes-the-electronic-properties-of-organic-solar-cells%2F&sa=D&sntz=1&usg=AFQjCNGLnKxzVv0NdcuXb5Vb25elogBz_w)**,**[**ORNL Review**](http://www.google.com/url?q=http%3A%2F%2Fweb.ornl.gov%2Finfo%2Fornlreview%2Fv47_1_14%2Farticle15.shtml&sa=D&sntz=1&usg=AFQjCNF7LV9Et4AIn8EHjB3xEi99h9bBEA)**,**[**ORNL News**](https://www.google.com/url?q=https%3A%2F%2Fwww.ornl.gov%2Fnews%2Fsolar-surprise&sa=D&sntz=1&usg=AFQjCNE7wSL1LgQ6BsZsUHSjGrQN-VqPTw)**.**
18. P. Hu, L. Wang, M. Yoon, J. Zhang, W. Feng, X. Wang, Z. Wen, J. C. Idrobo, Y. Miyamoto, D. B. Geohegan, K. Xiao\*, “Highly Responsive Ultrathin GaS Nanosheet Photodetectors on Rigid and Flexible Substrates”, Nano Lett. 13, 1649 (2013). **Note: Selected as a highlight by Nature Photonics, 7, 422 (2013).**
19. K. Xiao,\* W. Deng, J. K. Keum, M. Yoon, I. V. Vlassiouk, K.W. Clark, A. Li, I. I. Kravchenko, G. Gu, E. A. Payzant, B. G. Sumpter, S. C. Smith, J. F. Browning, D. B. Geohegan, “Surface- Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene”, J. Am. Chem. Soc., 135, 3680 (2013). **Note: Selected as a spotlight in JACS, 135, 3301 (2013).**
20. K. Xiao\*, M. Yoon, A. J. Rondinone, E. A. Payzant, and David B. Geohegan, “Understanding the Metal-Directed Growth of Single-Crystal M-TCNQF4 Organic Nanowires with Time- Resolved, in Situ X-ray Diffraction and First-Principles Theoretical Studies,” J. Am. Chem. Soc. 134, 14353 (2012) **Note: highlighted as the journal cover and selected as a spotlight article.**

**Full List of Publications**

186. W. Luo, A. D Oyedele, N. Mao, A. Puretzky, K. Xiao, L. Liang, X. Ling, [Excitation-Dependent Anisotropic Raman Response of Atomically Thin Pentagonal PdSe2](https://pubs.acs.org/doi/abs/10.1021/acsphyschemau.2c00007), ACS Physical Chemistry Au, 2(6), 482 (2022).

185. N. Li, A. Okmi, T. Jabegu, H. Zheng, K. Chen, A. Lomashvili, W. Williams, D. Maraba, I. Kravchenko, K. Xiao, K. He, S. Lei, van der Waals Semiconductor Empowered Vertical Color Sensor, ACS Nano, 16, 8619–8629 (2022).

184. A. Okmi, X. Xiao, Y. Zhang, R. He, O. Olunloyo, S. B Harris, T. Jabegu, N. Li, D. Maraba, Y. Sherif, O. Dyck, I. Vlassiouk, K. Xiao, P. Dong, B. Xu, S. Lei, Discovery of Graphene‐Water Membrane Structure: Toward High‐Quality Graphene Process, Advanced Science, 2201336 (2022).

183. K. Xiao, D. B. Geohegan, Laser synthesis and processing of atomically thin 2D materials, Trends in Chemistry, 4, 769(2022).

182. Y. Gu, L. Zhang, H. Cai, L. Liang, C. Liu, A. Hoffman, Y. Yu, A. Houston, A. A. Puretzky, G. Duscher, P. D. Rack, C. M. Rouleau, X. Meng, M. Yoon, D. B. Geohegan, Kai Xiao, Stabilized synthesis of 2D verbeekite: Monoclinic PdSe2 crystals with high mobility and in-plane optical and electrical anisotropy, ACS Nano. 16, 13900 (2022). **Note: This work was highlighted as the journal cover.**

181. T. Zheng, Y.-C. Lin, N. Rafizadeh, D. B. Geohegan, Z. Ni, K. Xiao, H. Zhao, Janus Monolayers for Ultrafast and Directional Charge Transfer in Transition Metal Dichalcogenide Heterostructures, ACS Nano 16, 4197-4205 (2022).

180. D. Zhou, M. Fuentes-Cabrera, A. Singh, R. R Unocic, J. M. Y Carrillo, K. Xiao, Y. Li, B. Li, Atomic Edge-Guided Polyethylene Crystallization on Monolayer Two-Dimensional Materials, Macromolecules, 55(2), 559 (2022).

179. W. Ko, Z. Gai, A. A Puretzky, L. Liang, T. Berlijn, J. A Hachtel, K. Xiao, P. Ganesh, M. Yoon, A.-P. Li, Understanding Heterogeneities in Quantum Materials, Advanced Materials, 2106909 (2022).

178. K. Wang, L. Zhang, G. D Nguyen, X. Sang, C. Liu, Y. Yu, W. Ko, R. R Unocic, A. A Puretzky, C. M Rouleau, D. B Geohegan,. Fu, G. Duscher, A.‐P. Li, M. Yoon, K. Xiao, Selective Antisite Defect Formation in WS2 Monolayers via Reactive Growth on Dilute W‐Au Alloy Substrates, Advanced Materials, 34(3), 2106674(2022). **Note: This work was highlighted as the journal Frontpieces.**

177. Y.-Y. Pai, C. E Marvinney, M. A Feldman, B. Lerner, Y. S. Phang, K. Xiao, J. Yan, L. Liang, J. Lapano, M. Brahlek, B. J Lawrie, Magnetostriction of α-RuCl3 Flakes in the Zigzag Phase, The Journal of Physical Chemistry C, 125 (46), 25687-25694 (2021).

176. Y. Guo, S. V Kalinin, H. Cai, K. Xiao, S. Krylyuk, A. V Davydov, Q. Guo, A. R Lupini, Defect detection in atomic-resolution images via unsupervised learning with translational invariance, npj Computational Materials, 7(1), 1-9 (2021).

175. J. Chen, S. Das, M. Shao, G. Li, H. Lian, J. Qin, J. F Browning, J. K Keum, D. Uhrig, G. Gu, K. Xiao, Phase segregation mechanisms of small molecule‐polymer blends unraveled by varying polymer chain architecture, SmartMat, 2(3), 367-377 (2021). **Note: This work was selected as the journal cover.**

174. C Liu, YC Lin, M Yoon, Y Yu, AA Puretzky, CM Rouleau, MF Chisholm, K. Xiao, G. Duscher, D. Geohegan, Understanding Substrate-Guided Assembly in van der Waals Epitaxy by in Situ Laser Crystallization within a Transmission Electron Microscope, ACS nano 15 (5), 8638-8652 (2021).

173. Y. Yu, G.S. Jung, C. Liu, YC Lin, C.M. Rouleau, M. Yoon, G. Eres, G. Duscher, K. Xiao, S. Irle, A. A Puretzky, D. B Geohegan, Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS2 Crystals, ACS nano 15 (3), 4504 (2021).

172. Y.‐C. Lin, R. Torsi, D. B. Geohegan, J. A. Robinson, K. Xiao, Controllable Thin‐Film Approaches for Doping and Alloying Transition Metal Dichalcogenides Monolayers, Adv. Sci., 2004249 (2021). **(Invited Review)**

171. T. Zheng, Y.-C. Lin, Y. Yu, P. Valencia-Acuna, A. A Puretzky, R. Torsi, C. Liu, I. N Ivanov, G. Duscher, D. B Geohegan, Z. Ni, K. Xiao, H. Zhao, Excitonic Dynamics in Janus MoSSe and WSSe Monolayers, Nano Lett., 21, 931 (2021).

170. Y. Liu, A. V. Levlev, N. Borodinov, M. Lorenz, K. Xiao, M. Ahmadi, B. Hu, S. V. Kalinin, O. S. Ovchinnikova, Direct Observation of Photoinduced Ion Migration in Lead Halide Perovskites, Advanced Functional Materials, 31, 2008777 (2021).

169. H. Cai, Y. Yu, Y.-C. Lin, A. A. Puretzky, D. B. Geohegan, K. Xiao, “Heterogeneities at multiple length scales in 2D layered materials: From localized defects and dopants to mesoscopic heterostructures”, Nano Research, 14, 1625 (2021). **Invited Review and Back cover.**

168. W. Luo, A. Oyedel, Y. Gu, T. Li, X. Wang, A. V. Haglund, D. Mandrus, A. A Puretzky, K. Xiao, L. Liang, X. Ling, “Anisotropic Phonon Response of few-Layer PdSe2 under Uniaxial Strain”, Advanced Functional Materials, 2003215 (2020).

167. K. Xiao, Z. Y. Al Balushi, S. Tongay, “Introduction of Focus Section: Heterogeneity in Beyond Graphene 2D Materials”, Journal of Materials Research 35 (11), 1349 (2020).

166. Y. Liu, M. Li, M. Wang, L. Collins, A. V Ievlev, S. Jesse, K. Xiao, B. Hu, A. Belianinov, O. S Ovchinnikova, “Twin domains modulate light-matter interactions in metal halide perovskites,” APL Materials 8, 11106 (2020).

165. A. Hoffman, Y. Gu, J. Tokash, J. Woodward, K. Xiao, P. D Rack, “Layer-by-layer thinning of PdSe2 flakes via Plasma Induced Oxidation and Sublimation”, ACS Applied Materials & Interfaces 12, 7345 (2020).

164. Y. Liu, A. V Ievlev, L. Collins, A. Belianinov, J. Keum, M. Ahmadi, S. Jesse, S. T Retterer, K. Xiao, J. Huang, “Strain–Chemical Gradient and Polarization in Metal Halide Perovskites”, Advanced Electronic Materials, 6(4), 1901235 (2020).

163. M. Fu, L. Liang, Q. Zou, G. D Nguyen, K. Xiao, A. Li, J. Kang, Z. Wu, Z. Gai, “Defects in Highly Anisotropic Transition-Metal Dichalcogenide PdSe2”, The Journal of Physical Chemistry Letters 11, 740-746 (2020).

162. K. A Dagnall, B. J Foley, S. A Cuthriell, M. R Alpert, X. Deng, A. Z Chen, Z. Sun, M. C Gupta, K. Xiao, S. Lee, “Relationship Between the Nature of Monovalent Cations and Charge Recombination in Metal Halide Perovskites”, ACS Applied Energy Materials 3, 1298 (2020).

161. G. D Nguyen, A. D Oyedele, A. Haglund, W. Ko, L. Liang, A. A Puretzky, D. Mandrus, K. Xiao, A. Li, “Atomically Precise PdSe2 Pentagonal Nanoribbons”, ACS nano 14 (2), 1951 (2020).

160. J. Ran, O. O Dyck, X. Wang, B. Yang, D. B Geohegan, K. Xiao, “Electron‐Beam‐Related Studies of Halide Perovskites: Challenges and Opportunities”, Advanced Energy Materials 10, 1903191 (2020).

159. A. A Puretzky, Y-C Lin, C. Liu, A. M Strasser, Y. Yu, S. Canulescu, C. M Rouleau, K. Xiao, G. Duscher, D. B Geohegan, “In situ laser reflectivity to monitor and control the nucleation and growth of atomically thin 2D materials”, 2D Materials 7(2), 25048 (2020).

158. Y-C. Lin, C. Liu, Y. Yu, E. Zarkadoula, M. Yoon, A. A Puretzky, L. Liang, X. Kong, Y. Gu, A. Strasser,… “Low Energy Implantation into Transition-Metal Dichalcogenide Monolayers to Form Janus Structures”, ACS nano 14(4), 3896(2020).

**Note: This work was selected as a DOE Office of Science “Science Headline”.**

157. Y. Gu, H. Cai, J. Dong, Y. Yu, A. N Hoffman, C. Liu, A. D Oyedele, Y‐C. Lin, Z. Ge, A. A Puretzky, G. Duscher, M. F Chisholm, P. D Rack, C. M Rouleau, Z. Gai, X. Meng, F. Ding, D. B Geohegan, K. Xiao, “Two‐Dimensional Palladium Diselenide with Strong In‐Plane Optical Anisotropy and High Mobility Grown by Chemical Vapor Deposition”, Advanced Materials 32(19), 1906238 (2020).

156. B. Doughty, M. J Simpson, S. Das, K. Xiao, Y. Ma, “Connecting Femtosecond Transient Absorption Microscopy with Spatially Co-Registered Time Averaged Optical Imaging Modalities,” The Journal of Physical Chemistry A 124, 3915 (2020).

155. X. Li, E. Kahn, G. Chen, X. Sang, J. Lei, D. Passarello, A. D Oyedele, D. Zakhidov, K. Chen, Y. Chen, et al “Surfactant-Mediated Growth and Patterning of Atomically Thin Transition Metal Dichalcogenides,” ACS Nano, 14, 6570 (2020).

154. Y. Gu, H. Cai, J. Dong, Y. Yu, A. N Hoffman, C. Liu, A. D Oyedele, Y. C Lin, Z. Ge, A. A Puretzky, G. Duscher, M. F Chisholm, P. D Rack, C. M Rouleau, Z. Gai, X. Meng, F. Ding, D. B Geohegan, K. Xiao, “2D Materials: Two‐Dimensional Palladium Diselenide with Strong In‐Plane Optical Anisotropy and High Mobility Grown by Chemical Vapor Deposition (Adv. Mater. 19/2020),” Advanced Materials, 32(19), 2070152 (2020).

**Note: This work was selected as the journal cover.**

153. N. N Hoffman, Y. Gu, L. Liang, J. D Fowlkes, K. Xiao, P. D Rack, “Exploring the air stability of PdSe2 via electrical transport measurements and defect calculations”, npj 2D Materials and Applications 3, 1-7 (2019).

152. H. Cai, Y. Gu, Y.-C. Lin, Y. Gu, D. B Geohegan, K. Xiao, “Synthesis and emerging properties of 2D layered III-VI metal chalcogenides”, Appl. Phys. Rev. 6, 04312 (2019).

151. J. Zhang, X. Li, K. Xiao, B. G Sumpter, A.W Ghosh, L. Liang, “The role of mid-gap phonon modes in thermal transport of transition metal dichalcogenides”, Journal of Physics: Condensed Matter 32 (2), 025306 (2019).

150. Y. Liu, L. Collins, R. Proksch, S. Kim, B. R Watson, B. Doughty, T. R Calhoun, et al. Reply to: On the ferroelectricity of CH3NH3PbI3 perovskites, Nature materials 18 (10), 1051-1053 (2019).

149. Y. Liu, A. V Ievlev, L. Collins, N. Borodinov, A. Belianinov, J. K Keum, M. Wang, M. Ahmadi, S. Jesse, K. Xiao, B. G Sumpter, B. Hu, S. V Kalinin, O. S Ovchinnikova, “Light‐Ferroic Interaction in Hybrid Organic–Inorganic Perovskites”, Advanced Optical Materials, 7, 1901451 (2019).

148. J. Wang, S. Senanayak, J. Liu, Y. Hu, Y. Shi, Z. Li, C. Zhang, B. Yang, L. Jiang, D. Di, A. Ievlev, O. Ovchinnikova, T. Ding, H. Deng, L. Tang, Y. Guo, J. Wang, K. Xiao, D. Venkateshvaran, L. Jiang, D. Zhu, H. Sirringhaus, “Investigation of Electrode Electrochemical Reactions in CH3NH3PbBr3 Perovskite Single‐Crystal Field‐Effect Transistors”, Advanced Materials 31, 1902618 (2019).

147. A. Oyedele, S. Yang, T. Feng, A. Haglund, Y. Gu, A. Puretzky, D. Briggs, C. Rouleau, M. Chisholm, R. Unocic, D. Mandrus, S. Pantelides, D. Geohegan, K. Xiao, “Defect-Mediated Phase Transformation in Anisotropic Two-Dimensional PdSe2 Crystals for Seamless Electrical Contacts”, J. Am. Chem. Soc. 141, 8928-8936 (2019).

146. K. Wang, A. A Puretzky, Z. Hu, B. R Srijanto, X. Li, N. Gupta, H. Yu, M. Tian, M. Mahjouri-Samani, X. Gao, A. Oyedele, C. Rouleau, G. Eres, B. Yakobson, M. Yoon, K. Xiao, D. B Geohegan, “Strain tolerance of two-dimensional crystal growth on curved surfaces”, Science Advances 5, eaav4028 (2019).

**Note: DOE Office of Science Highlight https://www.energy.gov/science/bes/articles/stretched-limit-and-sparkling-curved-surfaces.**

145. X. Sang, X. Li, A. A Puretzky, D. B Geohegan, K. Xiao, R. R Unocic, “Atomic Insight into Thermolysis‐Driven Growth of 2D MoS2”, Advanced Functional Materials 29, 1902149 (2019).

144. G.G Jiang, J. W Klett, J. McFarlane, A. Ievlev, K. Xiao, J. K Keum, M. Yoon, P. Im, M. Z Hu, J. E Parks, “Efficient Solar‐Thermal Distillation Desalination Device by Light Absorptive Carbon Composite Porous Foam”, Global Challenges, 1900003 (2019).

143. Y. Liu, A. Ievlev, L. Collins, A. Belianinov, S. Kim, B. Doughty, S. Jesse, M. Ahmadi, S. T Retterer, K. Xiao, B. G Sumpter, S. Kalinin, B. Hu, O. Ovchinnikova, “Multi-Model Imaging of Local Chemistry and Ferroic Properties of Hybrid Organic-Inorganic Perovskites”, Microscopy and Microanalysis, 25 (S2), 2076-2077 (2019).

142. D. B Brown, W. Shen, X. Li, K. Xiao, D. B Geohegan, S. Kumar, “Spatial Mapping of Thermal Boundary Conductance at Metal–Molybdenum Diselenide Interfaces”, ACS applied materials & interfaces 11 (15), 14418-14426 (2019)

141. M. G Stanford, Y.C. Lin, M. G Sales, A. N Hoffman, C. T Nelson, K. Xiao, S. McDonnell, P. D Rack, “Lithographically patterned metallic conduction in single-layer MoS2 via plasma processing”, npj 2D Materials and Applications 3 (1), 131(2019).

140. M. Zeng, Y. Chen, E. Zhang, J. Li, R. G.Mendes, X. Sang, S. Luo, W. Ming, Y. Fu, M. Du, L. Zhang, D. S. Parker, R. R.Unocic, K. Xiao, C. Wang, T. Zhang, Y. Xiao, M. H. Rümmeli, F. Xiu, L. Fu, “Molecular Scaffold Growth of Two-Dimensional, Strong Interlayer-Bonding-Layered Materials,” CCS Chemistry 1, 117 (2019).

139. A. Maksov, O. Dyck, K. Wang, K. Xiao, D. B Geohegan, B. G Sumpter, R. K Vasudevan, S. Jesse, S. V Kalinin, M. Ziatdinov, “Deep learning analysis of defect and phase evolution during electron beam-induced transformations in WS2”, npj Computational Materials 5 (1), 129 (2019).

138. X. Li, J. Zhang, A. A Puretzky, A. Yoshimura, X. Sang, Q. Cui, Y. Li, L. Liang, A. W Ghosh, H. Zhao, R. R Unocic, V. Meunier, C. M Rouleau, B. G Sumpter, D. B Geohegan, K. Xiao, “Isotope-Engineering the Thermal Conductivity of Two-Dimensional MoS2”, ACS Nano 13, 24812 (2019).

137. N. Briggs, S. Subramanian, Z. Lin, X. Li, X. Zhang, K. Zhang, K. Xiao, D. Geohegan, R. Wallace, L. Chen, M. Terrones, A. Ebrahimi, S. Das, J. Redwing, C. Hinkle, K. Momeni, A. Duin, V. Crespi, S. Kar, J. A Robinson, “A roadmap for electronic grade 2D materials”, 2D Materials 6, 0220019 (2019).

136. Y. Ma, B. Doughty, M. J Simpson, S. Das, K. Xiao, “On the origin of spatially dependent electronic excited-state dynamics in mixed hybrid perovskite thin films”, Lithuanian Journal of Physics 58 (4), 326-336 (2018)

135. R. Geng, R. C. Subedi, H. M. Luong, M. T. Pham, W. Huang, X. Li, K. Hong, M. Shao, K. Xiao, L. A. Hornak, T. T. Nguyen, “Effect of Electron Localization on the Effective Hyperfine Interaction in Organic Semiconducting Polymers”, Phys Rev Lett.120, 086602 (2018)

134. C. Zhang, P. Raj Pudasaini, A. D. Oyedele, A. V Ievlev, L. Xu, A. V Haglund, J. H Noh, A. T Wong, K. Xiao, T. Z Ward, D. Mandrus, H. Xu, O. S Ovchinnikova, P. D Rack, “Ion Migration Studies in Exfoliated 2D Molybdenum Oxide via Ionic Liquid Gating for Neuromorphic Device Applications”, ACS Applied Materials & Interfaces, 10, 22623 (2018).

133. X. Sang, Y. Xie, D. E Yilmaz, R. Lotfi, M. Alhabeb, A. Ostadhossein, B. Anasori, W. Sun, X. Li, K. Xiao, P. RC Kent, A. CT van Duin, Y. Gogotsi, R. R Unocic, “In situ atomistic insight into the growth mechanisms of single layer 2D transition metal carbides”, Nature Comm, 9, 2266 (2018).

132. X. Sang, X. Li, W. Zhao, J. Dong, C. M. Rouleau, D. B. Geohegan, F. Ding, K. Xiao, R. R. Unocic, “In situ edge engineering in two-dimensional transition metal dichalcogenides”, Nature Comm, 9, 2051 (2018).

131. A. A Puretzky, A. D Oyedele, K. Xiao, A. V Haglund, B. G Sumpter, D. Mandrus, D. B Geohegan, L. Liang, “Anomalous interlayer vibrations in strongly coupled layered PdSe2”, 2D Materials, 5, 035016 (2018).

130. B. Yang, W. Ming, M.-H. Du, J. K Keum, A. A Puretzky, C. M Rouleau, J. Huang, D. B Geohegan, X. Wang, K. Xiao, “Real-Time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites”, Advanced Materials, 30, 1705801 (2018).

129. M. Yarali, H. Brahmi, Z. Yan, X. Li, L. Xie, S. Chen, S. Kumar, M. Yoon, K. Xiao, A. Mavrokefalos, “The Effect of Metal Doping and Vacancies on the Thermal Conductivity of Monolayer Molybdenum Diselenide”, ACS Applied Materials & Interfaces, 10, 4921 (2018).

128. H. Li, X. Shan, J. N Neu, T. Geske, M. Davis, P. Mao, K. Xiao, T. Siegrist, Z. Yu, “Lead-free halide double perovskite-polymer composites for flexible X-ray imaging”, Journal of Materials Chemistry C 6 (44), 11961-11967 (2018).

127. M. Z Bellus, M. Mahjouri-Samani, S. D Lane, A. D Oyedele, X. Li, A. A Puretzky, D. Geohegan, K. Xiao, H. Zhao, “Photocarrier transfer across monolayer MoS2-MoSe2 lateral heterostructures”, ACS Nano, 12, 7086 (2018).

126. P. R. Pudasaini, A. Oyedele, C. Zhang, M. G Stanford, N. Cross, A.T Wong, A. N Hoffman, K. Xiao, G. Duscher, D. G Mandrus, T. Z Ward, P. D Rack, “High-performance multilayer WSe2 field-effect transistors with carrier type control”, Nano Research, 11, 772 (2018).

125. D. Xu, W. Chen, M. Zeng, H. Xue, Y. Chen, X. Sang, Y. Xiao, T. Zhang, R. Unocic, K. Xiao, L. Fu, “Crystal Field Tuning of Photoluminescence in Lanthanide Ions‐Embedded Two‐dimensional Materials”, Angewandte Chemie International Edition, 57, 755 (2018).

124. A. D. Oyedelea, C. M. Rouleau, D. B. Geohegan, K. Xiao, “The growth and assembly of organic molecules and inorganic 2D materials on graphene for van der Waals heterostructures”, Carbon, 131, 246 (2018).

123. Z. B Aziza, V. Zólyomi, H. Henck, D. Pierucci, M. Silly, J. Avila, S. Magorrian, J. Chaste, C. Chen, M. Yoon, K. Xiao, F. Sirotti, M. Asensio, E. Lhuillier, M. Eddrief, V. Fal’ko, A. R Ouerghi, “Valence band inversion and spin-orbit effects in the electronic structure of monolayer GaSe“, Phys Rev B 98, 115405 (2018).

122. W. Ko, S. M. Hus, X. Li, T. Berlijn, G. D. Nguyen, K. Xiao, A.-P. Li, “Tip-induced local strain on MoS2/graphite detected by inelastic electron tunneling spectroscopy”, PRB, 97, 125401 (2018).

121. J. Bauer, L. S Quintanar, K. Wang, A. A Puretzky, K. Xiao, D. B Geohegan, A. Boulesbaa, “Ultrafast Exciton Dissociation at the 2D-WS2 Monolayer/Perovskite Interface”, J. Phys. Chem. C 122, 28910-289173 (2018).

12o. N Briggs, MI Preciado, Y Lu, K Wang, J Leach, X Li, K Xiao, S Subramanian, B Wang, A Haque, S Sinnott, JA Robinson, “Transformation of 2D group-III selenides to ultra-thin nitrides: enabling epitaxy on amorphous substrates”, Nanotechnology 29 (47), 47LT021 (2018).

119. Y. Liu, L. Collins, R. Proksch, S. Kim, B. R Watson, B. Doughty, T. R Calhoun, M. Ahmadi, A. V Ievlev, S. Jesse, S. T Retterer, A. Belianinov, K. Xiao, J. Huang, B. G Sumpter, S. V Kalinin, B. Hu, O. S Ovchinnikova, ”Chemical nature of ferroelastic twin domains in CH3NH3PbI3 perovskite”, Nature Materials 17 (11), 1013-1019 (2018).

118. Y. Liu, L. Collins, A. Belianinov, S. M Neumayer, A. V Ievlev, M. Ahmadi, Kai Xiao, S. T Retterer, S. Jesse, S. V Kalinin, B. Hu, O. S Ovchinnikova, “Dynamic behavior of CH3NH3PbI3 perovskite twin domains”, Applied Physics Letters 113 (7), 072102 (2018).

117. X. Sang, X. Li, D. B Geohegan, K. Xiao, R. Unocic, “Atomistic Insights into Thermolysis and Growth of Two-Dimensional MoS2 Using In situ Electron Microscopy”, Microscopy and Microanalysis 24 (S1), 1568-1569 (2018).

116. G. D Nguyen, L. Liang, Q. Zou, M. Fu, A. D Oyedele, B. G Sumpter, Z. Liu, Z. Gai, K. Xiao, A. Li, “3D imaging and manipulation of subsurface selenium vacancies in PdSe2”, Phys Rev Lett 121, 086101 (2018).

115. A. N Hoffman, M. G Stanford, C. Zhang, I. N Ivanov, A. D Oyedele, M. G Sales, S. J McDonnell, M. R Koehler, D. G Mandrus, L. Liang, B. G Sumpter, K. Xiao, P. D Rack, “Atmospheric and Long-term Aging Effects on the Electrical Properties of Variable Thickness WSe2Transistors,” ACS applied materials & interfaces 10 (42), 36540-36548 (2018).

114. B. J Foley, S. Cuthriell, S. Yazdi, A. Z Chen, S. M Guthrie, X. Deng, G. Giri, S. Lee, K. Xiao, B. Doughty, Y. Ma, J. J Choi, “Impact of crystallographic orientation disorders on electronic heterogeneities in metal halide perovskite thin films”, Nano letters 18 (10), 6271-6278 (2018).

113. M. Ziatdinov, O. Dyck, A. Maksov, X. Li, X. Sang, K. Xiao, R. R Unocic, R. Vasudevan, S. Jesse, S. V Kalinin, “Deep Learning of Atomically Resolved Scanning Transmission Electron Microscopy Images: Chemical Identification and Tracking Local Transformations,” ACS Nano, 11 (12), pp 12742–12752 (2017).

112. X. Li, A. A. Puretzky, X. Sang, S. KC, M. Tian, F. Ceballos, M. Mahjouri-Samani, K. Wang, R. R. Unocic, H. Zhao, G. Duscher, V. R. Cooper, C. M. Rouleau, D. B. Geohegan, K. Xiao\*, “Suppression of Defects and Deep Levels Using Isoelectronic Tungsten Substitution in Monolayer MoSe2“, Advanced Functional Materials, 27, 1603850 (2017).

111. A. Oyedele, S. Yang, L. Liang, A. Puretzky, K. Wang, J. Zhang, P. Yu, P. Pudasaini, A. Ghosh, Z. Liu, C. Rouleau, B. Sumpter, M. Chisholm, W. Zhou, P. Rack, D. B. Geoghegan, K. Xiao,”PdSe2: Pentagonal 2D Layers with High Air Stability for Electronics” J. Am. Chem. Soc. 139, 14090 (2017).

**Note: DOE Office of Science Highlight https://science.osti.gov/bes/Highlights/2018/BES-2018-02-n**

110. H. Yu, N. Gupta, Z. Hu, K. Wang, B. R Srijanto, K. Xiao, D. B Geohegan, B. I Yakobson, “Tilt Grain Boundary Topology Induced by Substrate Topography”, ACS Nano, 11, 8612 (2017).

109. M. Mahjouri-Samani, M. Tian, A. A. Puretzky, M. Chi, K. Wang, G. Duscher, C. M. Rouleau, G. Eres, M. Yoon, J. C. Lasseter, K. Xiao, D. B. Geohegan, “Non-Equilibrium Synthesis of TiO2 Nanoparticle “Building Blocks” for Crystal Growth by Sequential Attachment in Pulsed Laser Deposition”, Nano Letters, 17, 4624 (2017).

108. M. G Stanford, P. R. Pudasaini, E. T. Gallmeier, L. Liang, N. Cross, A. Oyedele, G. Duscher, M. Mahjouri-Samani; K. Wang; K. Xiao; D. B. Geohegan; A. Belianinov, B. G. Sumpter, P. D. Rack, “High conduction hopping behavior induced in transition metal dichalcogenides by percolating defect networks: toward atomically thin circuits”, Advanced Functional Materials, 27, 1702829 (2017).

107. X Sang, D Yilmaz, Y Xie, M Alhabeb, B Anasori, X Li, K Xiao, PRC Kent, “Atomic Defects and Edge Structure in Single-layer Ti3C2Tx MXene”, Microscopy and Microanalysis 23 (S1), 1704-1705 (2017).

106. X. Li, J. Dong, J. C. Idrobo, A. A. Puretzky, C. M. Rouleau, D. B. Geohegan, F. Ding, K. Xiao, “Edge-controlled Growth and Etching of Two-Dimensional GaSe Monolayers”, J. Am. Chem. Soc. 139, 482 (2017).

105. M. J. Simpson, B. Doughty, S. Das, K. Xiao, Y.-Z. Ma, “Separating Bulk and Surface Contributions to Electronic Excited-State Processes in Hybrid Mixed Perovskite Thin Films via Multimodal All-Optical Imaging”, J. Phys. Chem. Lett., 8, 3299–3305 (2017).

104. Z. B. Aziza, D. Pierucci, H. Henck, M. G. Silly, C. David, M. Yoon, F. Sirotti, K. Xiao, M. Eddrief, J.-C. Girard, A. Ouerghi, “Tunable quasiparticle band gap in few-layer GaSe/graphene van der Waals heterostructures”, Phys. Rev. B 96, 035407 (2017).

103. P. R. Pudasaini, A. Oyedele, C. Zhang, M. G. Stanford, N. Cross, A. T. Wong, A. N. Hoffman, K. Xiao, G. Duscher, D. G. Mandrus, T. Z. Ward, P. D. Rack, “High-performance top-gated multilayer WSe2 field-effect transistors”, Nanotechnology, 28(47), 475202(2017).

102. LSL F. Wu, H. Un, Y. Li, H. Hu, Y. Yuan, B. Yang, K. Xiao, W. Chen, J.-Y Wang, J.‐Y. Wang, Z.‐Q. Jiang, J. Pei, L.‐S. Liao “An Imide-Based Pentacyclic Building Block for n-Type Organic Semiconductors”, Chemistry- A European Journal, 23(59), 14723(2017).

101. T. Tai, I. V. Kertesz, M.-W. Lin, B. R. Srijanto, D. K. Hensley, K. Xiao, G. J. Berkel, “Polymeric Spatial Resolution Test Patterns for Mass Spectrometry Imaging Using Nano-Thermal Analysis with Atomic Force Microscopy”, Rapid Communications in Mass Spectrometry, 31, 1204 (2017).

100. R. Guo, Z. Zhu, A. Boulesbaa, F. Hao, A. Puretzky, K. Xiao J. Bao, Y. Yao, W. Li, “Synthesis and photoluminescence properties of 2D phenethylammonium lead bromide perovskite nanocrystals”, Small Methods, 1(10), 1700245 (2017).

99. B. Yang, C. Brown, J. Huang, L. Collins, X. Sang, R. Unocic, S. Jesse, S. Kalinin, A. Belianinov, J. Jakowski, D. Geohegan, B. G. Sumpter, K. Xiao, O. S. Ovchinnikova, “Enhancing Ion Migration in Grain Boundaries of Hybrid Organic-Inorganic Perovskites by Chlorine”, Advanced Functional Materials, 27, 1700749 (2017).

98. A. Boulesbaa, V. E Babicheva, K. Wang, I. Kravchenko, M. W Lin, M. Mahjouri-Samani, C. B Jacobs, A. A Puretzky, K. Xiao, I. Ivanov, C. M Rouleau, D. B Geohegan, ”Ultrafast dynamics of metal plasmons induced by 2D semiconductor excitons in hybrid nanostructure arrays”, ACS Photonics 3 (12), 2389-2395 (2016).

97. Z. Lin, A. McCreary, N. Briggs, S. Subramanian, K. Zhang, Y. Sun, X. Li, N. Borys, H. Yuan, S. Fullerton-Shirey, A. Chernikov, H. Zhao, S. McDonnell, A. Lindenberg, K. Xiao, B. LeRoy, M. Drndić, J. Hwang, J. Park, M. Chhowalla, R. Schaak, A. Javey, M. Hersam, J. Robinson, M. Terrones, “2D Materials Advances: From Large Scale Synthesis and Controlled Heterostructures to Improved Characterization Techniques, Defects and Applications”, 2D Materials, 3, 042001 (2016).

96. A. Boulesbaa, K. Wang, M. Mahjouri-Samani, M. Tian, A. A Puretzky, I. Ivanov, C. M Rouleau, K. Xiao, B. G Sumpter, D. B Geohegan, ”Ultrafast charge transfer and hybrid exciton formation in 2D/0D heterostructures”, Journal of the American Chemical Society 138 (44), 14713-14719 (2016).

95. B. Yang, O. E Dyck, W. Ming, M.-H. Du, S. Das, C. M Rouleau, G. Duscher, D. B Geohegan, K. Xiao, "Observation of Nanoscale Morphological and Structural Degradation in Perovskite Solar Cells by In Situ TEM", ACS Applied Materials & Interfaces, 8, 32333 (2016).

94. X. Li, M.-W. Lin, L. Basile, S. M. Hus, A. A. Puretzky, J. Lee, Y.-C. Kuo, L.-Y. Chang, K. Wang, J. C. Idrobo, A.-P. Li, C.-H. Chen, C. M. Rouleau, D. B. Geohegan, K. Xiao\*, “Isoelectronic tungsten doping in monolayer MoSe2 for carrier type modulation”, Adv Mater, 28, 8240 (2016).

93. X. Li, M.-W. Lin, J. Lin, B. Huang, A. A. Puretzkya, C. Ma, K. Wang, W. Zhou, S. T. Pantelides, C. Miao, I. Kravchenko, J. Fowlkes, C. M. Rouleaua, D. B. Geohegan, K. Xiao\*, “Two- dimensional GaSe/MoSe2 misfit bilayer heterojunctions by van der Waals epitaxy”, Science Advances, 2, E1501882 (2016).

**Note: This work has been highlighted by**[***MRS Bulletin***](http://www.google.com/url?q=http%3A%2F%2Fjournals.cambridge.org%2Fdownload.php%3Ffile%3D%252FMRS%252FMRS41_07%252FS0883769416001445a.pdf%26code%3D72410e38b3b79e7f13924f0d065b8fde&sa=D&sntz=1&usg=AFQjCNHwBbZzzypep58jDhscNo-Jv72AxQ)**,**[***Photonics Spectra***](http://www.google.com/url?q=http%3A%2F%2Fwww.photonicsspectra-digital.com%2Fphotonicsspectra%2Fjune_2016%3Fpg%3D24%23pg24&sa=D&sntz=1&usg=AFQjCNENE2TkZrI0aOWUdC0EUqQdDCQNkw)**,**[***ORNL Press***](https://www.google.com/url?q=https%3A%2F%2Fwww.ornl.gov%2Fnews%2Fodd-couple-monolayer-semiconductors-align-advance-optoelectronics&sa=D&sntz=1&usg=AFQjCNE4zwYlICYOiqcwPKBXxcKikwMwrw)**, *Office of Science of DOE*,**[**ScienceDaily**](https://www.google.com/url?q=https%3A%2F%2Fwww.sciencedaily.com%2Freleases%2F2016%2F04%2F160415143756.htm&sa=D&sntz=1&usg=AFQjCNH3cN1qZgxeLRScdmDgdztTBR13GQ)**,**[**Phys.Org**](http://www.google.com/url?q=http%3A%2F%2Fphys.org%2Fnews%2F2016-04-odd-couple-monolayer-semiconductors-align.html&sa=D&sntz=1&usg=AFQjCNGtLvZSAgdHu14vY26_OSgTkFHu-g)**,**[***Optics and Photonics News***](http://www.google.com/url?q=http%3A%2F%2Fwww.osa-opn.org%2Fhome%2Fnewsroom%2F2016%2Fapril%2Fpairing_up_an_optoelectronic_mismatch%2F&sa=D&sntz=1&usg=AFQjCNGuYjakUP6g27BjioO8Y32THav5WQ)**,**[***AAAS EurekAlert***](http://www.google.com/url?q=http%3A%2F%2Fwww.eurekalert.org%2Fpub_releases%2F2016-04%2Fdrnl-cm041416.php&sa=D&sntz=1&usg=AFQjCNE-PQHWYBa9k6ParTbq6DDWNO3ZQg)**, et al.**

92. B. Yang, J. Keum, O. S. Ovchinnikova, A. Belianinov, S. Chen, M.-H. Du, I.N. Ivanov, C.M. Rouleau, D. B. Geohegan, K. Xiao\*, “Deciphering Halogen Competition in Organometallic Halide Perovskite Growth”. J. Am. Chem. Soc. 138, 5028 (2016).

91. B. Yang, M. Mahjouri-Samani, C. M. Rouleau, D. B. Geohegan, K. Xiao\*, “Pulsed Laser Deposition of Hierarchical TiO2 for High Performance Perovskite Solar Cells”, Physical Chemistry Chemical Physics, 18, 27067 (2016). PCCP themed issue: Physical chemistry of hybrid perovskite solar cells. (Invited)

90. S. Das, G. Gu, P. C. Joshi, B. Yang, T. Aytug, C. M Rouleau, D. Geohegan, K. Xiao\*, “Low Thermal Budget, Photonic-Cured Compact TiO2 Layer for High-Efficiency Perovskite Solar Cells”, J. Mater. Chem. A, 4, 8695 (2016).

89. X. Li, M.-W. Lin, A. A. Puretzkya, L. Basilea, K. Wang, J. C. Idroboa, C. M. Rouleaua, D. B. Geohegan, K. Xiao\*, “Persistent photoconductivity in two-dimensional Mo1−x Wx Se2–MoSe2 van der Waals heterojunctions”, J. Mater. Res. 31, 923 (2016). (**Invited for Focus Issue on “Two-Dimensional Heterostructure Materials**”)

88. M-W. Lin, I. Kravchenko, J. Fowlkes, X. Li, A. Puretzky, C. Rouleau, D. Geohegan, K. Xiao\*, "Thickness Dependent Charge Transport in Few-Layer MoS2 Field-Effect Transistors", Nanotechnology, 27, 165203 (2016).

87. M. Lin, H. L Zhuang, J. Yan, T. Z. Ward, A. A Puretzky, C. M Rouleau, Z. Gai, L. Liang, V. Meunier, B. G Sumpter, P. Ganesh, P. RC Kent, D. B Geohegan, D. G Mandrus, K. Xiao\*, “Ultrathin nanosheets of CrSiTe3: a semiconducting two-dimensional ferromagnetic material”, Journal of Materials Chemistry C, 4, 315 (2016).

86. W . Zheng, J. Lin, W. Feng, K. Xiao, Y. Qiu, X. Chen, G. Liu, W. Cao, S. T. Pantelides, W. Zhou P Hu, “Patterned Growth of P-Type MoS2 Atomic Layers Using Sol–Gel as Precursor”, Advanced Functional Materials, 26, 6371 (2016).

85. X. Sang, Y. Xie, M.-W. Lin, M. Alhabeb, K. L. Van Aken, Y. Gogotsi, P. R.C. Kent, K. Xiao, R. R. Unocic, “Atomic Defects in Monolayer Titanium Carbide (Ti3C2Tx) Mxene”, ACS Nano, 10, 9193 (2016).

84. M. Mahjouri-Samani, L. Liang, A. D. Oyedele, Y.-S. Kim, M. Tian, N. Cross, K. Wang, M.-W. Lin, A. Boulesbaa, C. M. Rouleau, A. A. Puretzky, K. Xiao, M. Yoon, G. Eres, G. Duscher, B. G. Sumpter, D. B. Geohegan, “Tailoring Vacancies Far Beyond Intrinsic Levels Changes the Carrier Type in Monolayer MoSe2-x Crystals”, Nano Lett., 16, 5213 (2016).

83. K. Wang, B. Huang, M. Tian, F. Ceballos, M.-W. Lin, M. Mahjouri-Samani, A. Boulesbaa, A. A Puretzky, C. M Rouleau, M. Yoon, H. Zhao, K. Xiao, G. Duscher, D. B Geohegan, “Interlayer Coupling in Twisted WSe2/WS2 Bilayer Heterostructures Revealed by Optical Spectroscopy”, ACS Nano, 10, 6612 (2016).

82. M. J. Simpson, B. Doughty, B. Yang, K. Xiao, Y.-Z. Ma, “Separation of Distinct Photoexcitation Species in Femtosecond Transient Absorption Microscopy”, ACS Photonics, 3, 434 (2016).

81. M. J. Simpson, B. Doughty, B. Yang, K. Xiao, Y.-Z. Ma, “Imaging electronic trap states in perovskite thin films with combined fluorescence and femtosecond transient absorption microscopy”, The journal of physical chemistry letters, 7, 1725 (2016).

80. B. Doughty, M. J. Simpson, B. Yang, K. Xiao, Y.-Z. Ma, “Simplification of femtosecond transient absorption microscopy data from CH3NH3PbI3 perovskite thin films into decay associated amplitude maps”, Nanotchnology, 27, 114002 (2016).

79. A. A. Puretzky, L. Liang, X. Li, K. Xiao, B. G. Sumpter, V. Meunier, D. B. Geohegan, “Twisted MoSe2 Bilayers with Variable Local Stacking and Interlayer Coupling Revealed by Low- Frequency Raman Spectroscopy”, ACS Nano, 10, 2736–2744 (2016).

78. N. Herath, S. Das, J. Zhu, R. Kumar, J. Chen, K. Xiao, G. Gu, J. F Browning, B. G Sumpter, I. N Ivanov, V. Lauter, “Unraveling the Fundamental Mechanisms of Solvent Additive-Induced Optimization of Power Conversion Efficiencies in Organic Photovoltaic Devices”, ACS Applied Materials & Interfaces, 8, 20220 (2016).

77. V. Iberi, L. Liang, A. V Ievlev, M. G Stanford, M.-W. Lin, X. Li, M. Mahjouri-Samani, S. Jesse, B. G Sumpter, S. V Kalinin, D. C Joy, K. Xiao, A. Belianinov, O. S. Ovchinnikova, “Nanoforging Single Layer MoSe2 Through Defect Engineering with Focused Helium Ion Beams”, Scientific Report, 6, 30481 (2016).

76. O. Dyck, S. Hu, S. Das, J. Keum, K. Xiao, B. Khomami, G. Duscher, “Quantitative Phase Fraction Detection in Organic Photovoltaic Materials through EELS Imaging”, Polymers, 7, 2446 (2015).

75. B. Yang, O. Dyck, J. Poplawsky, J. Keum, S. Das, A. Puretzky, T. Aytug, P. C. Joshi, C. M. Rouleau, G. Duscher, D, B. Geohegan, K, Xiao\*, “Controllable Growth of Perovskite Films by Room-Temperature Air Exposure for Efficient Planar Heterojunction Photovoltaic Cells,” Angewandte Chemie International Edition, 54, 14862 (2015).

74. B. Yang, O. Dyck, J. Poplawsky, J. Keum, A. Puretzky, S. Das, I. Ivanov, C. Rouleau, G. Duscher, D. Geohegan, and K. Xiao\*, "Perovskite Solar Cells with Near 100% Internal Quantum Efficiency Based on Large Single Crystalline Grains and Vertical Bulk Hetero-junctions", J. Am. Chem. Soc., 137, 9210 (2015).

**Note: The work was selected as a Science Highlight by Office of Sciences, U.S. Department of Energy, featured on DOE’s official website “**[**Problem Turned Into Performance for Solar Cells**](https://www.energy.gov/science/bes/articles/problem-turned-performance-solar-cells)**”, and released as a Research Highlight in August 2015 CNMS User Newsletter.**

73. D. Sanjib, B. Yang, G. Gu, P. Joshi, I. Ivanov, C. Rouleau, T. Aytug, D. Geohegan, K. Xiao\*, “High-Performance Flexible Perovskite Solar Cells by Using a Combination of Ultrasonic Spray-Coating and Low Thermal Budget Photonic Curing" ACS Photonics, 2, 680 (2015).

72. B. R. Watson, B. Yang, K. Xiao, Y.-Z. Ma, B. Doughty, T. R. Calhoun, “Elucidation of Perovskite Film Micro-Orientations Using Two-Photon Total Internal Reflectance Fluorescence Microscopy,” The Journal of Physical Chemistry Letters, 6, 3283 (2015).

71. M. J. Simpson, B. Doughty, B. Yang, K. Xiao, Y.-Z. Ma, “Spatial Localization of Excitons and Charge Carriers in Hybrid Perovskite Thin Films,” The Journal of Physical Chemistry Letters, 6, 3041 (2015).

70. A. K. Chilvery, A. K. Batra, B. Yang, K. Xiao, P. Guggilla, M. D. Aggarwal, R. Surabhi, R. B. Lal, J. R. Currie, B. G. Penn, “Perovskites: transforming photovoltaics, a mini-review,” J. Photon. Energy, 5, 057402 (2015).

69. N. Herath, S. Das, J. K Keum, J. Zhu, R. Kumar, I. N Ivanov, B. G Sumpter, J. F. Browning, K. Xiao, G. Gu, P. Joshi, S. Smith, V. Lauter, “Peculiarity of Two Thermodynamically-Stable Morphologies and Their Impact on the Efficiency of Small Molecule Bulk Heterojunction Solar Cells,” Scientific reports, 5, 13407 (2015).

68. S. Das, J. K. Keum, J. F. Browning, G. Gu, B. Yang, C. Do, W. Chen, J. Chen, I. N. Ivanov, K. Hong, A. J. Rondinone, P. C. Joshi, D. B. Geohegan, K. Xiao\*, “Correlating High Power Conversion Efficiency of PTB7:PC71BM Inverted Organic Solar Cells to Nanoscale Structure,” Nanoscale, 7, 1551 (2015).

67. B. Wang, R. Sun, D. D. Günbaş, H. Zhang, F. C. Grozema, K. Xiao and S. Jin, “A bundled-stack discotic columnar liquid crystalline phase with inter-stack electronic coupling”, Chem Comm, 51, 11387 (2015).

66. X. Li, L. Basile, M. Yoon, C. Ma, A. A. Puretzky, J. Lee, J. C. Idrobo, M. Chi, C. M. Rouleau, D. B. Geohegan, and K. Xiao\*, “Revealing the Preferred Interlayer Orientations and Stackings of Two-Dimensional Bilayer Gallium Selenide Crystals,” Angewandte Chemie International Edition, 54, 2712 (2015)

65. X. Li, L. Basile, B. Huang, C. Ma, J. Lee, I. V. Vlassiouk, A. A. Puretzky, M.-W. Lin, M. Yoon, M. Chi, J. C. Idrobo, C. M. Rouleau, B. G. Sumpter, D. B. Geohegan, K. Xiao, “Van der Waals Epitaxial Growth of Two-Dimensional Single-Crystalline GaSe Domains on Graphene”, ACS Nano, 9, 8078 (2015).

64. M. Mahjouri-Samani, M.-W. Lin, K. Wang, A. R. Lupini, J. Lee, L. Basile, A. Boulesbaa, C. M. Rouleau, A. A. Puretzky, I. N. Ivanov, K. Xiao, M. Yoon, D. B. Geohegan, "Patterned Arrays of Lateral Heterojunctions within Monolayer 2D Semiconductors", Nature Comm. 6, 7749 (2015).

63. A. Boulesbaa, B. Huang, K. Wang, M.-W. Lin, M. Mahjouri-Samani, C. Rouleau, K. Xiao, M. Yoon, B. Sumpter, A. Puretzky, D. Geohegan, “Observation of two distinct negative trions in tungsten disulfide monolayers,” Physical Review B, 92, 115443 (2015).

62. W. Feng, J.-B. Wu, X. Li, W. Zheng, X. Zhou, K. Xiao, W. Cao, B. Yang, W. Tian, P. Tan, P. Hu, “Broadband InSe Nanosheet Photodetectors: Thickness Optimization, Simultaneously Ultrahigh Photo-responsivity and Detectivity”, J. Mater. Chem. C, 3, 7022 (2015).

61. L.D. Casto, A. J. Clune, J. L. Musfeldt, T. J. Williams, H. L. Zhuang, R. G. Hennig, M.-W. Lin, K. Xiao, B. B. Sales, J.-Q. Yan, D. Mandrus, “Strong Spin-Lattice Coupling in CrSiTe3,” APL Materials, 3, 041515 (2015).

60. A.A. Puretzky, L. Liang, X. Li, K. Xiao, K. Wang, M. Mahjouri-Samani, L. Basile, J. C. Idrobo, B. G. Sumpter, V. Meunier, D. B. Geohegan, “Low-Frequency Raman Fingerprints of Two- Dimensional Metal Dichalcogenide Layer Stacking Configurations”, ACS Nano, 9, 6333 (2015).

59. M. Mahjouri-Samani, M. Tian, K. Wang, A. Boulesbaa, C. M Rouleau, A. A Puretzky, M. Alan McGuire, B. R Srijanto, K. Xiao, G. Eres, G. Duscher, D. Geohegan, “Digital Transfer Growth of Patterned 2D Metal Chalcogenides by Confined Nanoparticle Evaporation”, ACS Nano, 8, 11567 (2014).

58. M. Shao, J. K. Keum, R. Kumar, J. Chen, J. F. Browning, S. Das, W. Chen, J. Hou, C. Do, K. C. Littrell, A. Rondinone, D. B. Geohegan, B. G. Sumpter, K. Xiao\*, “Understanding how processing additives tune the nanoscale morphology of high efficiency organic photovoltaic blends: From casting solution to spun-cast thin film”, Adv. Funct. Mater., 24, 6467 (2014).

57. M. Mahjouri-Samani, R. Gresback, M. Tian, A. A. Puretzky, C. M. Rouleau, G. Eres, I. N. Ivanov, K. Xiao, M. McGuire, G. Duscher, D. B. Geohegan, “Pulsed Laser Deposition of Photoresponsive GaSe Nanosheet Networks”, Adv. Funct. Mater., 24, 6365 (2014).

56. X. Li, M.-W. Lin, A. A. Puretzky, J. C. Idrobo, C. Ma, M. Chi, M. Yoon, C. M. Rouleau, I. I. Kravchenko, D. B. Geohegan, K. Xiao,\* “Controlled Vapor Phase Growth of Single Crystalline, Two-Dimensional GaSe Crystals with High Photoresponse”, Sci. Rep. 4, 5497 (2014).

55. P. Hu, J. Zhang, M. Yoon, W. Feng, P. Tan,W. Zheng, J. Liu, X. Wang, J. C. Idrobo, D. B. Geohegan, K. Xiao,\* “Highly Sensitive Phototransistors Based on Two-Dimensional GaTe Nanosheets with Direct Bandgap”, Nano Research, 7, 694 (2014).

54. M. Shao, J. Keum, J. Chen, Y. He, W. Chen, J. F. Browning, J. Jakowski, B. G. Sumpter, I. N. Ivanov, Y. Ma, C. M. Rouleau,4S. C. Smith, D. B. Geohegan, K. Hong, K. Xiao,\* "The isotopic effects of deuteration on the optoelectronic properties of conducting polymers", Nature Comm. 5, 4180 (2014). **Note: The work was selected as a Science Highlight by Office of Sciences, U.S. Department of Energy, featured on DOE’s official website, and released as a Research Highlight by**[**Materials Views**](http://www.google.com/url?q=http%3A%2F%2Fwww.materialsviews.com%2Fdeuterium-changes-the-electronic-properties-of-organic-solar-cells%2F&sa=D&sntz=1&usg=AFQjCNGLnKxzVv0NdcuXb5Vb25elogBz_w)**,**[**ORNL Review**](http://www.google.com/url?q=http%3A%2F%2Fweb.ornl.gov%2Finfo%2Fornlreview%2Fv47_1_14%2Farticle15.shtml&sa=D&sntz=1&usg=AFQjCNF7LV9Et4AIn8EHjB3xEi99h9bBEA)**,**[**ORNL News**](https://www.google.com/url?q=https%3A%2F%2Fwww.ornl.gov%2Fnews%2Fsolar-surprise&sa=D&sntz=1&usg=AFQjCNE7wSL1LgQ6BsZsUHSjGrQN-VqPTw)**.**

53. J. Chen, M. Shao, K. Xiao, A. J. Rondinone, Y.-L. Loo, J. E. Anthony, P. R. C. Kent, B. G. Sumpter, J. Huang, “Solvent-Type-Dependent Crystalline Polymorphism of High Performance Small Molecule Organic Semiconductor Thin Films Fabricated by Slow Solution Crystallization”, Nanoscale 6, 449 (2014).

52. J. Keum, J. F. Browning, K. Xiao, M. Shao, C. E. Halbert, K. Hong, “Morphological origin for the stratification of P3HT:PCBM blend film studied by neutron reflectometry”, Appl. Phys. Lett. 103, 223301 (2013).

51. J. Chen, M. Shao, K. Xiao, Z. He, D. Li, B. S. Lokitz, D. Hensley, S. M. Kilbey II, J. E. Anthony, A. J. Rondinone, Z. Bao, “Conjugated Polymer-Mediated Polymorphism of High Performance, Small-Molecule Organic Semiconductor with Tuned Intermolecular Interactions, Enhanced Long-Range Order and Charge Transport”, Chem. Mater. 25, 4378 (2013).

50. Y. He, M. Shao, K. Xiao, S. Smith, K. Hong, "High-Performance Polymer Photovoltaics with Rationally Designed Fullerene Acceptors", Solar Energy Materials and Solar Cells 118, 171 (2013)

49. A.Mohsin,L.Liu,P.Liu,W.Deng,I.Ivanov,G.Duscher,J.Dunlap,K.Xiao,G.Gu “Synthesis of Millimeter-Size Hexagon-Shaped Graphene Single Crystals on Resolidified Copper”, ACS Nano, 7, 8924 (2013).

48. M. Shao, S. Das, J. Chen, J. K. Keum, I. N. Ivanov, G. Gu, W. Durant, D. Li, D. B. Geohegan, K. Xiao\*, “High-Performance Organic Field-Effect Transistors with Dielectric and Active Layers Printed Sequentially by Ultrasonic Spraying”, J Mater Chem C 1, 4384 (2013).

47. P. Hu, L. Wang, M. Yoon, J. Zhang, W. Feng, X. Wang, Z. Wen, J. C. Idrobo, Y. Miyamoto, D. B. Geohegan, K. Xiao\*, “Highly Responsive Ultrathin GaS Nanosheet Photodetectors on Rigid and Flexible Substrates”, Nano Lett. 13, 1649 (2013). \*

**Note: Selected as a highlight by Nature Photonics, 7, 422 (2013).**

46. H. Chen, J. Chen, W. Yin, X. Yu, M. Shao, K. Xiao, K. Hong, D. L. Pickel, W. M. Kochemba, S. M., Kilbey, M. Dadmun, “Correlation of Polymeric Compatibilizer Structure to its Impact on the Morphology and Function of P3HT:PCBM Bulk Heterojunctions”, J. Mater. Chem. A, 1, 5309 (2013). \*

45. K. Xiao,\* W. Deng, J. K. Keum, M. Yoon, I. V. Vlassiouk, K.W. Clark, A. Li, I. I. Kravchenko, G. Gu, E. A. Payzant, B. G. Sumpter, S. C. Smith, J. F. Browning, D. B. Geohegan, “Surface- Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene”, J. Am. Chem. Soc., 135, 3680 (2013).

**Note: Selected as a spotlight in JACS, 135, 3301 (2013).**

44. M. Shao, Y. He, K. Hong, C. M. Rouleau, D. B. Geohegan, and K. Xiao, “A Water-Soluble Polythiophene for Organic Field-Effect Transistors”, Polymer Chemistry, 4, 5270, (2013). (Invited paper)

43. S. Wu, W. Li, M. Lin, Q. Burlingame, Q. Chen, A. Payzant, K. Xiao, and Q. M. Zhang, “Aromatic Polythiourea Dielectrics with Ultrahigh Breakdown Field Strength, Low Dielectric Loss, and High Electric Energy Density,” Adv. Mater. 25, 1734 (2013).

42. J. Keum, K. Xiao, I. N Ivanov, K. Hong, J. Browning, G. Smith, M. Shao, K. C Littrell, A. Rondinone, E. A. Payzant, J. Chen, D. K. Hensley, “Solvent Quality-Induced Nucleation and Growth of Parallelepiped Nanorods in Dilute Poly(3-Hexylthiophene) (P3HT) Solution and the Impact on the Crystalline Morphology of Solution-Cast Thin Film”, CrystEngComm 15, 1114 (2013).

41. S. Wu, M. Shao, Q. Brulingame, X. Chen, M. Lin, K. Xiao, Q. Zhang, “A high-K ferroelectric relaxor terpolymer as a gate dielectric for organic thin film transistors,” Appl. Phys. Lett. 102, 013301 (2013).

40. Y. Ma, K. Xiao, and R.W. Shaw, Exciton–Exciton Annihilation in Copper-phthalocyanine Single-Crystal Nanowires,” J. Phys. Chem. C 116, 21588−21593 (2012).

39. K. Xiao\*, M. Yoon, A. J. Rondinone, E. A. Payzant, and David B. Geohegan, “Understanding the Metal-Directed Growth of Single-Crystal M-TCNQF4 Organic Nanowires with Time- Resolved, in Situ X-ray Diffraction and First-Principles Theoretical Studies,” J. Am. Chem. Soc. 134, 14353 (2012)

**Note: highlighted as the journal cover and selected as a spotlight article.**

38. R. Hegde, N. Henry, B. Whittle, H. Zang, B. Hu, J. Chen, K. Xiao, M. Dadmun, “The impact of controlled solvent exposure on the morphology, structure and function of bulk heterojunction solar cells,” Solar Energy Materials and Solar Cells, 107, 112 (2012).

37. P. Hu, Z. Wen, L. Wang, P. Tan, K. Xiao,\* “Synthesis of Few-Layer GaSe Nanosheets for High Performance Photodetectors,” ACS Nano 6, 5988 (2012).

36. J. Chen, X. Yu, K. Hong, J. M. Messman, D. L. Pickel, K. Xiao, M. D. Dadmun, J. W. Mays, A. J. Rondinone, B. G. Sumpter, S. M. Kilbey II, “Ternary behavior and systematic nanoscale manipulation of domain structures in P3HT/PCBM/P3HT-b-PEO films,” J. Mater. Chem. 22, 13013 (2012).

35. Z. He, K. Xiao, D. Durant, J. E. Anthony, K. Hong, S. M. Kilbey, II, J. Chen, and D. Li, “Enhanced Performance Consistency in Nanoparticle/TIPS Pentacene-Based Organic Thin Film Transistors,” Advanced Functional Materials 19, 3617 (2011).

34. L. Luo, C. Wilhelm, C. N. Young, C. P. Grey; G. P. Halada, K. Xiao, I. N. Ivanov, and J. Y. Howe, D. B. Geohegan, N. Goroff, “Characterization and Carbonization of Highly Oriented Poly(diiododiacetylene) Nanofibers,” Macromolecules 44, 2626 (2011).

33. Z. Sun; K. Xiao,\* J. K. Keum, X. Yu, K. Hong, I. Ivanov, J. Chen, D. Li, B. Sumpter, A. Payzant, C. Rouleau, and D. B. Geohegan, “PS-b-P3HT Copolymers as P3HT/PCBM Interfacial Compatibilizers for High Efficiency Photovoltaics,” Advanced Materials 23, 5529 (2011).

32. X. Yu, K. Xiao,\* J. Chen, N. V. Lavrik, K. Hong, B. G. Sumpter, and D. B. Geohegan, “High- Performance Field-Effect Transistors Based on Polystyrene-b-Poly(3-hexylthiophene) Diblock Copolymers,” ACS Nano 5, 3559 (2011).

31. M. A. Schreuder, K. Xiao, I. N. Ivanov, S. M. Weiss, and S. J. Rossenthal, “White Light- Emitting Diodes Based on Ultrasmall CdSe Nanocrystal Electroluminescence,” Nano Letters 10, 573 (2010).

30. K. Xiao,\* R. Li, J. Tao, E. A. Payzant, I. N. Ivanov, A. A. Puretzky, W. Hu, and D. B. Geohegan, “Metastable Copper-Phthalocyanine Single-Crystal Nanowires and Their Use in Fabricating High-Performance Field-Effect Transistors,” Advanced Functional Materials 19, 3776 (2009).

29. K. Xiao,\*A. J. Rondinone, A. A. Puretzky, I. N. Ivanov, S. T. Retterer, and D. B. Geohegan, “Growth, Patterning, and One-Dimensional Electron-Transport Properties of Self-Assembled Ag-TCNQF(4) Organic Nanowires,” Chemistry of Materials 21, 4275 (2009).

28. R. Aggarwal, R. J. Narayan, K. Xiao, and D. B. Geohegan, “Fabrication of Ag- Tetracyanoquinodimethane Nanostructures Using Ink-jet Printing/Vapor-Solid Chemical Reaction Process,” Journal of Vacuum Science and Technology B 26(6), L48 (2008).

27. Z. Liu, D. J. Styers-Barnett, A. A. Puretzky, C. M. Rouleau, D. Yuan, I. N. Ivanov, K. Xiao, and D. B. Geohegan, “Pulsed Laser CVD Investigations of Single-Wall Carbon Nanotube Growth Dynamics,” Applied Physics A 93, 987 (2008).

26. K. Xiao\*, J. Tao, A. A. Puretzky, I. N. Ivanov, S. T. Retterer, S. J. Pennycook and D. B. Geohegan, “Selective Patterned Growth of Single-crystal Organic Nanowires of Ag-TCNQ by Vapor-Solid Chemical Reaction,” Advanced Functional Materials 18, 3043 (2008).

25. K. Xiao, Y. Fu, Y. Liu, G. Yu, J. Zhai, L. Jiang, W. Hu, Z. Shuai, Y. Luo, and D. Zhu, “Photo- Electrical Characteristic of C/CNx Multi-Walled Nanotube,” Advanced Functional Materials 17, 2842 (2007).

24. K. Xiao,\* J. Tao, Z. Pan, A. A. Puretzky, I. N. Ivanov, S. J. Pennycook, and D. B. Geohegan, “Single-Crystal Organic Nanowires of Cu-TCNQ: Synthesis, Patterning, Characterization and Device Applications,” Angewandte Chemie International Edition 46, 2650 (2007).

23. Z. Zhou, K. Xiao, R. Jin, D. Mandrus, J. Tao, D. B. Geohegan, and S. Pennycook, “One- Dimensional Electron Transport in Cu-TCNQ Organic Nanowires,” Applied Physics Letters 90, 193115 (2007).

22. Y. Sun, Y. Ma, Y. Liu, Y. Lin, Z. Wang, Y. Wang, C. Di, K. Xiao, X. Chen, W. Qiu, B. Zhang, G. Yu, W. Hu, and D. Zhu, “High-Performance and Stable Organic Thin-Film Transistors Based on Fused Thiophenes,” Advanced Functional Materials 16, 426 (2006).

21. K. Xiao,\* I. N. Ivanov, A. A. Puretzky, Z. Liu, and D. B. Geohegan, “Directed Integration of TCNQ-Cu Organic Nanowires Growth into Device Fabrication,” Advanced Materials 18, 2184 (2006).

20. K. Xiao, Y. Liu, P. Hu, G. Yu, W. Hu, D. Zhu, X. Liu, H. Liu, and D. Wu, “Electronic Transport Characteristics of an Individual CNx/C Nanotube Schottky Junction,” Applied Physics A: Materials Science & Processing 83, 53 (2006).

19. Y. Sun, Y. Ma, Y. Liu, Y. Lin, Z. Wang, Y. Wang, C. Di, K. Xiao, X. Chen, W. Qiu, B. Zhang, G. Yu, W. Hu, and D. Zhu, “High-Performance and Stable Organic Thin-Film Transistors Based on Fused Thiophenes,” Advanced Functional Materials 16, 426 (2006).

18. W. Su, J. Jiang, K. Xiao, Y. Chen, Q. Zhao, G Yu, and Y. Liu, “Thin-Film Transistors Based on Langmuir-Blodgett Films of Heteroleptic Bis(phthalocyaninato) Rare Earth Complexes”, Langmuir 21, 6527 (2005).

17. Y. M. Sun, K. Xiao, Y. Q. Liu, J. Wang, J. Pei, G. Yu, and D. B. Zhu, “Oligothiophene-Functionalized Truxene: Star-Shaped Compounds for Organic Field-Effect Transistor,” Advanced Functional Materials 15, 818 (2005).

16. K. Xiao, Y. Liu, Y. G. Guo, G. Yu, L. Wan, and D. Zhu, “Influence of the Self-Assembly Monolayers on the Characteristics of Copper Phthalacyanine Thin Film Transistor,” Applied Physics A: Materials Science & Processing 80, 1541 (2005).

15. K. Xiao, Y. Liu, T. Qi, W. Zhang, F. Wang, J. Gao, W. Qiu, Y. Ma, G. Cui, S. Chen, X. Zhan, G. Yu, J. Qin, W. Hu, and D. Zhu, “A Highly π-Stacked Organic Semiconductor for Field-Effect Transistors Based on Linearly Condensed Pentathienoacene,” Journal of the American Chemical Society 127, 13281 (2005). (Top 20 papers published in 2004-2007, Thomson Science Watch; Time cited: 190)

14. K. Xiao, Y. Q. Liu, P. A. Hu, G. Yu, Y. M. Sun, and D. B. Zhu, “n-Type Field-Effect Transistor Made of an Individual Nitrogen-Doped Multi-walled Carbon Nanotube,” Journal of the American Chemical Society 127, 8614 (2005).

13. P. Hu, K. Xiao, Y.Q. Liu, G. Yu, X.B. Wang, L. Fu, and D. B. Zhu, “Multi-Wall Nanotubes with Intratube Junctions (CNx/C): Preparation, Rectification, Logic Gates and their Application as a Wave-Detector in Transistor Radio Set”, Applied Physics Letter 84, 4932 (2004).

12. L. Fu, Y. Liu, P. Hu, K. Xiao, G. Yu, and D. Zhu, “Ga2O3 Nanoribbons: Synthesis, Characterization and Electronic Properties,” Chemistry of Materials 15, 4287 (2003).

11. K. Xiao, Y. Q. Liu, P. A. Hu, G. Yu, X. B. Wang, and D. B. Zhu, “High-Mobility Thin-Film Transistors Based on Aligned Carbon Nanotubes,” Applied Physics Letters 83, 150 (2003). Appears also in Virtual Journal of Nanoscale Science & Technology 8(2) (2003). (http://www.vjnano.org/)

10. K. Xiao, Y. Q. Liu, X. B. Huang, Y. Xu, G. Yu, and D. B. Zhu, “Field-Effect Transistors Based on Langmuir-Blodgett Films of Phthalocyanine Derivatives as Semiconductor Layers,” Journal of Physical Chemistry B 107, 9226 (2003).

9. K. Xiao, Y. Q. Liu, P. A. Hu, G. Yu, L. Fu, and D. B. Zhu, “High Performance Field-Effect Transistors made of Multiwall CNx/C Nanotube Intramolecular Junction,” Applied Physics Letters 83, 4824 (2003). Appears also in Virtual Journal of Nanoscale Science & Technology 8(12), (2003). http://www.vjnano.org/, (2003).

8. K. Xiao, Y. Liu, G. Yu, and D. Zhu, “Influence of the Substrate Temperature During Deposition on Film Characteristics of Copper Phthalocyanine and Field-Effect Transistor Properties,” Applied Physics A: Materials Science & Processing 77, 367 (2003).

7. K. Xiao, Y. Q. Liu, G. Yu, and D. B. Zhu, “Organic Field-Effect Transistors Using Copper Phthalocyanine Thin Film,” Synthetic Metals 137, 991 (2003).

6. X. B. Wang, Y. Q. Liu, P. A. Hu, G. Yu, K. Xiao, and D. B. Zhu, “Controllable Fabrication of Three-Dimensional Carbon Nanotube Alignments,” Advanced Materials 14(21), 557 (2002).

5. K. Xiao, Y. Q. Liu, G. Yu, and D. B. Zhu, “Organic Field-Effect Transistors,” Chinese Science Bulletin 47, 881 (2002). In Chinese

4. K. Xiao, Y. G. Yan, L. C. Lei, Y. L. Du, “Application of Pd-Ag Alloy Diffusion Anode for Electrochemical Hydrogen Sensor,” Corrosion Science and Protection Technology 14, 125 (2002). In Chinese

3. L. C. Lei, K. Xiao, Y. Shen, X. Shi, Y. Gao, Y. L. Du, “Preparation and Characteristics of A Novel Imidazoline Inhibitor Made from Naphthenic Acid and Diethy-lenetriamine,” Corrosion and Protection 22, 420 (2001). In Chinese

2. K. Xiao, Y. G. Yan, L. C. Lei, and Y. L. Du, “Studies of Solid State Electrolyte Hydrogen Sensors,” Corrosion Science and Protection technology 13,165 (2001). In Chinese

1. J. R. Song, Z. X. Gong, M. B. Luo, and K. Xiao, “Study on the Performance of Adsorbing Uranium by Attapulgite Clay,” Journal of East China Geological Institute 21, 265 (1998). In Chinese

**Patents:**

2017 D. B. Geohegan, O. E. Dyck, J. K. Keum, J. D. Poplawsky, K. Xiao, B. Yang, “Hybrid Perovskite Films”, 20170098514.

2015 D. B. Geohegan, M-W. Lin, M. Mahjouri-Samani, A. Puretzky, C. M. Rouleau, K. Wang, K. Xiao, “Patterned Two-Dimensional Heterocrystals”, 201503565, DOE S-138,201

2003 Y. Q. Liu, K. Xiao, P. A. Hu, G. Yu, L. Fu, D. B. Zhu, “A New Method for the Fabrication of Nanotube-FET Devices Based on N-doped Carbon Nanotubes,” CN ZL 03108244.

2003 Y. Q. Liu, K. Xiao, P. A. Hu, G. Yu, L. Fu, D.B. Zhu, “Process for Preparing a CNx/C Nanotube Diodes and Its Rectifying Properties,” CN ZL 03104280.5.

2004 Y. Q. Liu, Y. Sun, Y. Ma, K. Xiao, G. Yu, D. Zhu, “Fabrication Way and Application of 5,5’-bis-biphenyl-dithieno[3,2-b:2’,3’-d]thiophene Compounds,” CN ZL 200410046350.8.

2004 Y. Q. Liu, K. Xiao, Y. Fu, G. Yu, Y. Luo, J. Zhai, L. Jiang, W. Hu and D. Zhu, “Fabrication Way of Field-Effect Transistors Controlled by Light Intensity,” CN ZL 200410101837.1.

2002 Y.Q. Liu, K. Xiao, P.A. Hu, G. Yu, X. B. Wang, D. B. Zhu, “Fabrication of Thin-Film Transistors Based on Aligned Carbon Nanotubes,” CN ZL 02145889.8.

2002 Y. Q. Liu, P. A. Hu, K. Xiao, X. B. Wang, L. Fu, D. B. Zhu, “Fabrication and Application of CNx/C Nanotube Junctions,” CN ZL 02160815.6.

2002 Y. Q. Liu, X. B. Wang, P. A. Hu, G. Yu, K. Xiao, and D. B. Zhu, “A Synthesis Method of Three-Dimensional Carbon Nanotube Alignments,” CN ZL 02102542.8.

**Presentations:**

50. “Understanding the van der Waals epitaxial growth of 2D materials and heterostructures”, 2023 Lawrence Symposium on Epitaxy, Arizona State University, Phoenix, AZ, January 5-6, 2023. (Invited talk)

49. “Isotope effect on the thermal and optical properties of atomically thin 2D materials”, the 20th International Symposium on the Physics of Semiconductors and Applications (ISPSA 2022), Jeju, Korea, July 17~21, 2022 (Invited talk)

48. “Nonequilibrium synthesis to tailor heterogeneity in 2D materials”, the Guadalupe Workshop X on single wall carbon nanotubes and related materials, Hill Country, TX, May 13-17, 2022. (Invited talk)

47. “Defect Engineering in 2D Materials by Non-equilibrium Synthesis and Processing”, International Conference on Advances in Functional Materials (AAAFM-UCLA), August, 18-20, 2021, virtual (Invited talk)

46. “In situ x-ray and neutron diffraction studies of crystallization mechanism and phase transformation of hybrid perovskites”, Materials Synthesis Science and Opportunities Aided by in-situ Scattering Tools Workshop in the 2021 Joint Nanoscience and Neutron Scattering User Meeting, August 9-12, 2021 (Invited talk)

45. “2D Materials for Interconnects”, Creating Helpful Incentives to Produce Semiconductors (CHIPS) for America Act, ORNL Internal Lab Strategy Workshop, July 7–8, 2021 (invited talk)

44. “Tailoring Synthesis and Assembly of 2D Materials for Monolayer and Bilayer heterostructures”, Virtual MRS Spring/Fall meeting, Nov 27-Dec 4, 2020. (Invited talk)

43. “Tailoring the optoelectronic functionality of 2D materials by non-equilibrium synthesis and processing”, The Northrop Grumman/Brookhaven Lab Workshop, May 5-5, 2021. (Invited talk)

42. “Defect-Mediated Phase Transformations in Highly Anisotropic 2D Quantum Materials”, CNMS User Meeting, Oak Ridge, Aug 10-12, 2020.

41. “Tailoring the Heterogeneities in 2D Materials by Controlled Synthesis and Processing”, AVS 66th International Symposium & Exhibition, Columbus, Ohio, October 20-25, 2019.

40. “Toward Synthetic Control over Heterogeneity and Functionality in Two-Dimensional Materials”, 2019 Synthesis and Processing Science Principal Investigators’ Meeting, Gaithersburg Marriott Washingtonian Center, Gaithersburg, MD, July 17-19, 2019.

39. “The shape of things to come for 2D materials: a pentagonal layered PdSe2 for electronics”, 2019 Graphene & Beyond workshop, Penn State University, State College, PA, May 8-10, 2019.

38. “The Effect of Doping, Vacancies and Isotopes on the Thermal Conductivity of 2D Materials”, MRS Spring Meeting, Phoenix, Arizona, April 22-26, 2019.

37. “Defect-Induced Phase Transformation in Low-Symmetry 2D Materials for High Performance Electronics”, MRS Spring Meeting, Phoenix, Arizona, April 22-26, 2019. (contributed talk).

36. “Tailoring the heterogeneities in 2D materials by controlled synthesis and processing”, The TMS 148th Annual Meeting and Exhibition, Mar 10-14, 2019, San Antonio, Texas. (Invited talk).

35. “Strain-Engineered Growth of 2D Materials on Patterned Substrates”, MRS Spring Meeting, Phoenix, Arizona, April 2-6, 2018.

34. “Tailoring the heterogeneity in 2D materials for optoelectronics”, XXVII International Materials Research Congress, Cancun, Mexico, August 19-24, 2018.

33. “Toward Synthetic Control over Heterogeneity and Functionality in Two-Dimensional Materials”, 2017 Synthesis and Processing Science Principal Investigators’ Meeting, Gaithersburg Marriott Washingtonian Center, Gaithersburg, MD November 7-9, 2017.

32. “Heterogeneity in 2D Materials: From Localized Defects, Isoelectronic Doping to Macroscopic Heterostructures”,The 64th AVS International Symposium and Exhibition, Oct 29-Nov 3, 2017, Tampa, Florida. (Invited talk)

31. “Defect engineering in two dimensional materials”, The 7th International Conference on Nanoscience & Nanotechnology, China 2017, August 29-31, Beijing, China. (Invited talk)

30. “2D materials research at ORNL”, Synthesis and Collective Phenomena in 2D and Layered Materials Workshop at 2017 Joint Nanoscience and Neutron Scattering User Meeting, Oak Ridge, TN, July 31, 2017. (Invited talk)

29. “Edge-Controlled Growth and Etching of Two-Dimensional Materials”, 9th International Conference on Materials for Advanced Technologies (ICMAT), Suntec Singapore, June 18-23, 2017. (Invited talk)

28. “Defect Engineering in Monolayer MoSe2 through Controlled Synthesis and Doping”, MRS Spring Meeting, Phoenix, AZ, April 16-21, 2017. (Invited talk)

27. “Understanding the Growth of 2D Materials for Optoelectronic Devices”, Guadalupe workshop on Nucleation and Growth Mechanisms of Atomically-Thin Nanomaterials: From SWCNTs to 2D Crystals”, San Antonio, Texas, April 21-25, 2017.

26. “Epitaxial Growth and Optoelectronic Properties of 2D Materials”, International Graphene Innovation Conference, Qingdao, China, September 22-24, 2016. (Invited talk).

25. “Heterogeneity in 2D systems: From localized defects to macroscopic van der Waals heterostructures”, CNMS User Meeting Workshop: Collective Phenomena in Layered and 2D Materials, Oak Ridge, TN, August 9-10, 2016. (Invited talk)

24. “Controlled synthesis and processing of perovskite films for high-efficiency Organometal Halide Perovskite Photovoltaics”, IUMRS-International Conference on Electronic Materials, Suntec, Singapore, July 4-8, 2016. (Invited talk)

23. “Isoelectronic Doping of MoSe2 Monolayers for 2D Heterostructures”, IUMRS-International Conference on Electronic Materials, Suntec, Singapore, July 4-8, 2016. (Invited talk)

22. “Understanding the Effect of Solvent Additive on Nanophase Engineering in Organic Photovoltaics”, The 30th Chinese Chemical Society (CCS) Congress, Dalian, China, July 1-4, 2016. (Invited talk)

21. “Isoelectronic Doping of MoSe2 Monolayers for 2D Heterostructures”, Graphene and Beyond workshop, Penn State University, State College, PA, May 9-10, 2016. (Invited talk)

20. “Ultrasonic Spray Printing for High-Performance Flexible Organic Field-Effect Transistors and Hybrid Perovskite Solar Cells”, The 145th TMS Annual Meeting & Exhibition, Recent Advancement on Stretchable and Wearable Electronics, Nashville, TN, February 14-18, 2016. (Invited talk)

19. “Synthesis, processing, and optoelectronic devices of van der Waals heterostructures”, The 40th International Conference and Exposition on Advanced Ceramics and Composites, Daytona Beach, FL, January 24-29, 2016. (Invited talk)

18. “Van der Waals Epitaxial Growth of Atomically Thin Lattice-misfit GaSe/MoSe2 Heterostructures”, the 2nd International Conference on Two-Dimensional Layered Materials, Hong Kong, January 7-9, 2016. (Invited talk)

17. “Synthesis of Two-Dimensional Metal Chalcogenides by Laser Vaporization and CVD”, 2015 Synthesis and Processing Science Principal Investigators’ Meeting, Washington DC North/Gaithersburg, Gaithersburg, MD, November 2-4, 2015.

16. “Understanding the effect of deuterated conducting polymer and solvent additive on the performance of organic photovoltaics”, SNS/HFIR 2015 User Meeting, Oak Ridge, October 26-27, 2015.

15. “Effect of Isoelectronic Doping on the Optoelectronic Properties of MoSe2 Monolayer Crystals”, The 6th International Conference on Nanoscience & Technology, Beijing, China, Sep. 3-5, 2015. (Invited talk)

14. “Understanding the Effect of Solvent Additive on the Performance of Organic Photovoltaics”, 23rd World Forum on Advanced Materials, Lincoln, Nebraska, May 11-15, 2015. (Invited talk)

13. “Revealing the Origin of High-Efficiency in Layer-by-Layer Processed Organometal Halide Perovskite Photovoltaics”, MRS spring conference, San Francisco, April 7-12, 2015.

12. “The Isotopic Effects of Deuteration on the Charge Transport and Optoelectronic Properties of Conducting Polymers,” XXIII International Materials Research Congress, August 17 – 21, 2014, Cancún, Mexico. (Invited talk)

11. “Synthesis and Properties of Two-Dimensional Layered Metal-Chalcogenides and their Heterostructures,” International Symposium on “Materials Chemistry of Two-Dimensional Crystals, at Peking University, Beijing, China, August 5-6, 2014. (Invited talk)

10. “The isotopic effects deuteration on the optoelectronic properties of conducting polymers,” American Conference on Neutron Scattering, Knoxville, TN, USA, June 1-5, 2014.

9. “Substrate-mediated assembly and growth of organic semiconductor nanostructures,” The 5th International Conference on Nanoscience & Technology, Beijing, China, Sep. 5-7, 2013. (Invited talk)

8. “Understanding the metal-directed growth of semiconducting organic nanocrystals,” Joint NSRC Workshop on Nanoparticle Science, November 5-6, 2012 Argonne National Laboratory.

7. “Isotope Effect of Deuterated P3HT on Charge Transport and Solar Harvesting,” International Conference on Science and Technology of Synthetic Metals, Atlanta, Georgia, July 8-13, 2012.

6. “Self-Assembly of Conjugated Block Copolymers for Organic Field-Effect Transistors and Photovoltaics,” The 10th Int. Symposium on Functional π-Electron Systems, Beijing, China, Oct. 13, 2011.

5. “Self-Assembled Single Crystal Organic Nanowires for High-performance Memory Devices,” Workshop on Self-Assembled Organic Nanomaterials: Structure and Function at The Molecular Foundry, Lawrence Berkeley National Laboratory, San Francisco, CA, Oct. 5-6, 2011.

4. “Block Copolymer Controlled Morphology of P3HT/PCBM Photovoltaics,” 4th Workshop on Sustainable Energy Future: Nanomaterials Enabled Photovoltaics, ORNL, Oak Ridge, TN, Sept. 22-23, 2011.

3. “Tailored Assemblies of PS-b-P3HT Diblock Copolymers: Adaptable Building Blocks for High-Performance Organic Transistors and Solar Cells”, 2011 EBMC-NSRC Contractors’ Meeting, Annapolis, MD, May 31, 2011.

2. “One-Dimensional Electron-Transport in Self-Assembled Organic Nanowires,” 9th International Symposium on Functional π-Electron Systems, Atlanta, GA, Oct. 6, 2010

1. “Synthesis of Organic Semiconductor Nanowires for Solar Cells”, 3th Workshop on Sustainable Energy Future: Nanomaterials Enabled Photovoltaics, ORNL, Oak Ridge, TN, Sept. 22, 2010.

**University Colloquium and Seminar**

11. “Tailoring the heterogeneities in 2D materials by non-equilibrium synthesis and processing”, Physics Colloquium, School of Science and Engineering, Tulane University, October 31, 2022.

10. “Synthetic strain engineering in 2D materials”, Mechanic Engineering Department Colloquium, Villanova University, November 13, 2020.

9. “Heterogeneity in 2D materials: synthesis and functionality”, Department of Physics and Astronomy Colloquium, Georgia State University, November 10, 2020.

8. “Toward Synthetic Control over Heterogeneity and Functionality in 2D Quantum Materials”, CNMS Seminar, Oak Ridge, TN, March 10, 202o.

7. “Tailoring the heterogeneity in 2D materials for optoelectronics and quantum information science” at the University of Tennessee at Knoxville – Department of Materials Science & Engineering – Materials Seminar, Knoxville, TN, October 8, 2019.

6. “Heterogeneity in 2D Materials: From Localized Defects to Macroscopic Heterostructures”, Department of Physics & Astronomy, Vanderbilt University, Jan 18, 2018.

5. “2D materials: synthesis and functionality”, College of Engineering, University of Georgia, October 23, 2017.

4. “Controlled Synthesis and Processing of Organometal Halide Perovskite Thin Film for high-efficiency Photovoltaics”, Department of Physics and Astronomy, University of Georgia, Athens, October 29, 2015.

3. “Heterogeneity in 2D systems: From Doped Monolayers to van der Waals Heterostructures”, Physical Sciences Directorate Chemical and Materials Sciences Seminar, ORNL, Oak Ridge, November 18, 2015.

2. “Twisted Bilayer and Tri-layer Two-Dimensional Metal Chalcogenides: Controlled Synthesis, Characterization, and Optoelectronic Devices”, Department of Mechanical Engineering, University of Houston, February 12, 2015

1. “Two-dimensional Chalcogenide Crystals: Synthesis, Characterization, and Optoelectronics”, Department of Materials Science and Engineering Seminar, University of Tennessee, Knoxville, March 7, 2014.

**Professional Activities: (International Conference and Workshop Organizer, Editorial and Conference Board, Review and Service)**

2023 Steering committee member of 17th International Conference on Laser Ablation (COLA)

2023 Program committee of AVS 69th International Symposium & Exhibition

2022 Sectary of the AVS 2D Materials Technical Group (2DMTG) Executive Council

2021 Organizing committee member of ORNL workshop for CHIPS Act

2021 Special Issue: Nanocarbon-Based Biosensors” in journal Biosensors, co-editor with Liming Huang and Kenneth Hunter

2020 The Focus Section: Heterogeneity in Beyond Graphene 2D Materials in Journal Material Research, Vol35, issue 11, June 2020. Co-editor with Zakaria Y. Al Balushi and Sefaattin Tongay).

2020 International Advisory Committee Member for the Centre for Advanced Electronics at Indian Institute of Technology (IIT) Indore.

2019 A CAREER panel review for EPMD (Electronics, Photonics and Magnetic Devices) program, NSF.

2018 Emerging 2D Non-Graphene Materials in XXVII International Materials Research Congress (IMRC2018). Co-organizer: Deji Akinwande (University of Texas at Austin), and Talat Rahman (University of Central Florida)

2018 International Advisory Committee of the International Conference on Computational Mathematics in Nanoelectronics and Astrophysics (CMNA 2018), India

2018 The committee member of the ‘2D Materials Focus Topic’ Program Committee for the AVS 65th International Symposium & Exhibition.

2017 Synthesis and Collective Phenomena in 2D and Layered Materials workshop in 2017 Joint Nanoscience and Neutron Scattering User Meeting, 2017. (Co-organizer with David Mandrus and Travis Williams).

2008-present Journal Editorial Board: Scientific Report; AIMS Materials Science.

**Proposal reviewer**: NSF Reviewer Panels on Organic Electronics, Materials Engineering and Processing (MEP) Program and Photonic Devices, Electronics, Photonics and Magnetic Devices (EPMD) program; DOE-BES; The European Research Council (ERC); The Netherlands Dutch Research Council (NWO); the Czech Science Foundation and Israel Science Foundation. ORNL seeds and LDRD; User proposal reviewer for the Molecular Foundry at Laurence Berkeley National laboratory and Stanford Synchrotron Radiation Lightsource (SSRL).

**Journal Reviewer:** Nature, Nature Mater; Nature Nano; Nature Chem; Nature Photonics; Nature Comm.; Light: Science & Applications; NPG Asia Materials; Scientific Report; J. Am. Chem. Soc.; Nano Letters, J. Phys. Chem. B; Chem. Mater.; ACS Nano; Langmuir; Angew. Chem. Int. Ed.; Adv. Mater.; Adv. Func. Mater.; Adv. Energy Mater.; Small; ChemSusChem; PCCP; Chem. Eur. J; Appl. Phys. Lett.; Phys Rev Lett; Phys Rev B; Phys Rev Mater; Nanoscale; J. Mater. Chem.; Polymer Chemistry; Polymer Reviews; J. Appl. Polymer Sci.; 2D Materials; Materials Today

**Professional Society Membership:** Materials Research Society (MRS)**,** American Vacuum Society (AVS).

**Honors and Awards:**

2021 The Nano Research Young Innovators (NR45) Awards in two-dimensional materials

2020 UT-Battelle Outstanding Scholarly Output

2017 CNMS Distinguished Scientific Paper Award

2014 CNMS Distinguished Scientific Paper Award

2007 The National Top 100 Excellent Ph. D. Thesis Award in China, Ministry of Education

2006 The Top 50 Excellent Ph. D. Thesis Award of the Chinese Academy of Sciences

2004 Outstanding Thesis Award of the 24th Annual Meeting, Chinese Chemical Society

**Graduate and Postdoctoral Advisors:**

Profs. Daoben Zhu and Yunqi Liu, Institute of Chemistry, Chinese Academy of Sciences (PhD Advisor)

Dr. David B Geohegan, Oak Ridge National Laboratory (Postdoc Advisor)

**Postdoctoral Researcher Advised:**

1. Dr. Yiling Yu (2019-2021) Now faculty at Wuhan University
2. Dr. Yu-Chuan Lin (2017-2020) Now faculty at National Taiwan University
3. Dr. Hui Cai (2018-2020) Now faculty at University of California at Merced
4. Dr. Ben Foley (IC Postdoc, 2018-2019) now at Covalent Metrology
5. Dr. Xufan Li (2013-2017) Now Senior scientist at Honda Research Center
6. Dr. Kai Wang (2014-2018) Now working at Intel Corporation
7. Dr. Ming-Wei Lin (2013-2016) Now working at Texas A&M University
8. Dr. Bin Yang (2015-2018) Now Professor at Hunan University
9. Dr. Ming Shao (2013-2015) Now Professor at Huazhong University of Science and Technology

**Ph.D. Students Advised:**

1) Mr. Olugbenga Olunloyo (UTK, 2019-present).

2) Ms. Yiyi Gu (visiting student from Technical Institute of Physics and Chemistry, CAS, 2017-2019)

3) Mr. Akinola Oyedele (UTK, 2014-2018) Now working at The Boston Consulting Group (BCG).

4) Mr. Sanjib Das (UTK, 2011-2016) Now Process Technology Engineer at Intel Corporation.