

Kai Xiao, Ph.D.

Senior R&D Staff Scientist
Functional Hybrid Nanomaterials Group
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

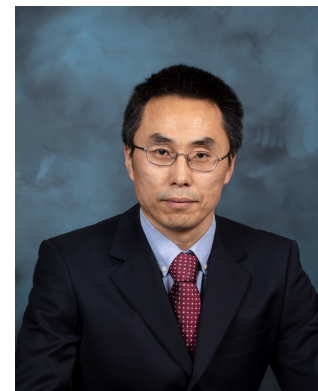
[Website](#) [Google Scholar](#)

Education:

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

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

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



Research Expertise:

- ~ 20 Years Research Experience in functional nanomaterial synthesis, characterization, and devices.
- Expertise in the synthesis and processing of functional nanomaterials including CVD, PVD, exfoliation, and other approaches.
- Expertise in the in-situ characterization of materials synthesis and processing by x-ray diffraction 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 Materials, conjugated polymers, halide perovskites.

Research and Professional Experience:

2018- Present	Senior R&D Staff Scientist	Oak Ridge National Laboratory
2011- Present	Joint faculty in EE	University of Tennessee Knoxville
2014- Present	Joint Faculty in Bredesen Center	University of Tennessee Knoxville
2013-2017	R&D Staff Scientist	Oak Ridge National Laboratory
2008-2013	R&D Associate	Oak Ridge National Laboratory
2005-2008	Postdoctoral Research Associate	Oak Ridge National Laboratory (Mentor: David B Geohegan)

Patents:

- 2015 D. B. Geohegan, M-W. Lin, M. Mahjouri-Samani, A. Puzetky, C. M. Rouleau, K. Wang, K. Xiao, "Patterned Two-Dimensional Heterocrystals", 201503565, DOE S-138,201
- 2017 D. B. Geohegan, O. E. Dyck, J. K. Keum, J. D. Poplawsky, K. Xiao, B. Yang, "Hybrid Perovskite Films", 20170098514.
- 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 CN_x/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 CN_x/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.

Funding:

- 2018- Present DOE Office of Science, BES Materials Science and Engineering Division. "Growth Mechanisms and Controlled Synthesis of Nanomaterials". (David Geohegan) (Xiao, Co-PI)

- 2018- present 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)
- 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. B. Yang, M.J. 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, Springer Series on Nanoscience and Nanotechnology, Vol. 7, 2018, pp 33-60.
2. B. Yang, D. B. Geohegan, K. Xiao, "Perovskite Materials: Solar Cells and Optoelectronic Applications" in Encyclopedia of Inorganic and Bioinorganic Chemistry, ed R. A. Scott, John Wiley: Chichester. DOI: 10.1002/9781119951438. Published 15 March 2017.
3. 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.
4. David B. Geohegan, Alex A. Puzos, Mina Yoon, Gyula Eres, Chris Rouleau, Kai Xiao, Jeremy Jackson, Jason Readle, Murari Regmi, Norbert Thonard, Gerd Duscher, Matt Chisholm and Karren 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.
5. D. B. Geohegan, A. A. Puzos, 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).
6. 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: [h index as of 07/03/2020: h-52 (google scholar)]

168. W. Luo, A. Oyedele, Y. Gu, T. Li, X. Wang, A. V. Haglund, D. Mandrus, A. A Puzos, 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 levlev, 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 levlev, 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 Cuthrell, 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 Puzos, 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 Puzos, 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 Puzos, 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 Puzetzy, 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 Puzetzy, 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, Reply to: On the ferroelectricity of CH₃NH₃PbI₃ perovskites, *Nature materials* 18 (10), 1051-1053 (2019).
149. Y. Liu, A. V levlev, 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-Ferroc 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. levlev, 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. Puzetzy, 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 Puzetzy, 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 Puzetzy, 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. levlev, 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. levlev, 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 Ferroc 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. Rummeli, 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 Puzetzy, 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 levlev, 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. Alhabeab, 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 Puzetky, 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 Puzetky, 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 Puzetky, 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. Oyedele, 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 Puzetky, 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).
120. 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 levlev, 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 levlev, 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 WSe₂ Transistors," *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. Puzetky, 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. Puzetky, K. Wang, J. Zhang, P. Yu, P. Pudasaini, A. Ghosh, Z. Liu, C. Rouleau, B. Sumpter, M. Chisholm, W. Zhou, P. Rack, D. B. Geohegan, 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. Puzetky, 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 Alhabeab, B Anasori, X Li, K Xiao, PRC Kent, "Atomic Defects and Edge Structure in Single-layer Ti₃C₂T_x MXene", *Microscopy and Microanalysis* 23 (S1), 1704-1705 (2017).
106. X. Li, J. Dong, J. C. Idrobo, A. A. Puzetky, 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. Puzetky, 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 Puzetky, 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 Puzetzky, I. Ivanov, C. M Rouleau, K. Xiao, B. G Sumpter, D. B Geohegan, "Ultrafast charge transfer and hybrid exciton formation in 2D/oD 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. Puzetzky, 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. Puzetzky, C. Ma, K. Wang, W. Zhou, S. T. Pantelides, C. Miao, I. Kravchenko, J. Fowlkes, C. M. Rouleau, 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, Photonics Spectra, ORNL Press, Office of Science of DOE, ScienceDaily, Phys.Org, Optics and Photonics News, AAAS EurekAlert, 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. Puzetzky, L. Basilea, K. Wang, J. C. Idrobo, C. M. Rouleau, D. B. Geohegan, K. Xiao*, "Persistent photoconductivity in two-dimensional Mo_{1-x}W_xSe₂-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. Puzetzky, 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 Puzetzky, 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. Alhabeab, K. L. Van Aken, Y. Gogotsi, P. R.C. Kent, K. Xiao, R. R. Unocic, "Atomic Defects in Monolayer Titanium Carbide (Ti₃C₂T_x) 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. Puzetzky, 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 Puzetzky, 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", *Nanotechnology*, 27, 114002 (2016).
79. A. A. Puzetzky, 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. Puzetzy, 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. Puzetzy, 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", 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. Puzetzy, 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. Vlasiouk, A. A. Puzetzy, 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. Puzetzy, 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. Puzetzy, 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. Puzetzy, 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. Puzetzy, 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. Puzetzy, 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. Puzetky, 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, 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).
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. Vlassiuk, 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. Burlingame, 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. Rosenthal, "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. Puzetky, 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. Puzetky, I. N. Ivanov, S. T. Retterer, and D. B. Geohegan, "Growth, Patterning, and One-Dimensional Electron-Transport Properties of Self-Assembled Ag-TCNQ(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. Puzetky, 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. Puzetky, 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. Puzetky, 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. Puzetky, 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 Phthalocyanine 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 (CN_x/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 CN_x/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 Attapulgitic Clay," *Journal of East China Geological Institute* 21, 265 (1998). In Chinese

Presentations:

42. "Tailoring Synthesis and Assembly of 2D Materials for Monolayer and Bilayer heterostructures", MRS Spring meeting, Phoenix, Arizona, April 14, 2020 and also as Session Chair at 2D Materials Symposium. (Postponed).
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.
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

8. "Toward Synthetic Control over Heterogeneity and Functionality in 2D Quantum Materials", CNMS Seminar, Oak Ridge, TN, March 10, 2020.
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)

- 2020 The Focus Section: Heterogeneity in Beyond Graphene 2D Materials in JMR, Vol35, issue 11, June 2020. Co-organized with Zakaria Y. Al Balushi and Sefaattin Tongay).
- 2018 Emerging 2D Non-Graphene Materials in XXVII International Materials Research Congress (IMRC2018). Lead Symposium Organizer. Deji Akinwande (University of Texas at Austin), and Talat Rahman (University of Central Florida) (Co-organizers)
- 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).

Editorial and Conference Board, Review and Service:

- 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 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.
- 2012 Organic Electronics program, Proposal Review Panelist.
- 2008-present Journal Editorial Board: Scientific Report; AIMS Materials Science.
- 2008-present Proposal Reviewer: NSF Reviewer Panel on Organic Electronics, Materials Engineering and Processing Program (MEP), DOE-BES, ORNL seeds and LDRD, User proposal reviewer for the Molecular Foundry at Lawrence Berkeley National laboratory and Stanford Synchrotron Radiation Lightsource (SSRL).
- 2008-present Journal Reviewer: Nature, Nature Nano; 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.; 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).

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. Hui Cai (Oak Ridge National Laboratory 2018-Present).
- 2) Dr. Ben Foley (IC Postdoc, ORNL, 2018-2019) now at Covalent Metrology
- 3) Dr. Xufan Li (ORNL, 2013-2017) Now Senior scientist at Honda Research Center.
- 4) Dr. Kai Wang (ORNL, 2014-2018) Now working at Intel Corporation.
- 5) Dr. Ming-Wei Lin (ORNL, 2013-2016) Now working at Texas A&M University.
- 6) Dr. Bin Yang (Oak Ridge National Laboratory 2015-2018) Now Professor at Hunan University
- 7) Dr. Ming Shao (Oak Ridge National Laboratory 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.