

Kai Xiao

R&D Staff
Functional Hybrid Nanostructures Group
Center for Nanophase Materials
Oak Ridge National Laboratory
Joint faculty
Bredesen Center and Department of Electrical
Engineering and Computer Sciences, University of
Tennessee, Knoxville (UTK)
(865) 574-7690
xiaok@ornl.gov



Education

East China Institute of Technology, China	Chemistry	B.A., 1998
Institute of Metal Research, Chinese Acad. of Sci., China	Material Science & Engr.	M. S., 2001
Institute of Chemistry, Chinese Acad. of Sci., China	Physical Chemistry	Ph. D., 2004

Professional Experience

2008–p Research Staff Member, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory (ORNL)
2011–p Joint faculty, Bredesen Center and Department of Electrical Engineering and Computer Sciences, University of Tennessee, Knoxville (UTK)
2005–2008 Postdoctoral Research Associate, Center for Nanophase Materials Sciences, ORNL

Professional and Synergistic Activities

Proposal Reviewer:

NSF Reviewer Panel on Organic Electronics, Materials Engineering and Processing Program (MEP), DOE-BES proposal reviewer, User proposal reviewer for the Molecular Foundry at Lawrence Berkeley National laboratory and Stanford Synchrotron Radiation Lightsource (SSRL).

Editorial Board: *Scientific Report*; *AIMS Materials Science*

Journal Reviewer: *Nature Nanotechnology*; *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.*; *Two-Dimensional Materials*; *Materials Today*.

Honors and Awards

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

Research Synopsis:

My research focused on the functional nanomaterials and their energy-related applications. Research Interests: organic and conducting polymer processing and self-assembly, low dimensional materials (including 1D, 2D) synthesis and processing, electron transfer and transport in nanomaterials and at the interface, thin film and nanoscale electronic and photonic devices, solar cells, and chemical sensors.

1. *Two-dimensional (2D) nanomaterials, including transition metal dichalcogenides and graphene.*

Synthesis of 2D nanomaterials and their van der Waals heterostructures using CVD, PVD, mechanical exfoliation, and dry transfer methods; Optical, structural, and electrical characterization of 2D

nanomaterials; 2D electronic and photonic devices; Understanding the critical roles of heterogeneity, interfaces, and disorder in 2D nanomaterials.

2. ***Solution-processed thin film electronic devices for organic semiconductors and hybrid perovskites, including field-effect transistors (FETs) and photovoltaics (PVs), spin valves, organic memory, sensors.***
Optical and optoelectronic characterization of solution-processed semiconductor materials (small molecules, conducting polymers, and hybrid perovskites); Processing those materials using various methods, including spin-coating, thermal deposition, spray printing, to form gradient or doped single/multilayer thin films for energy-related electronic devices (OFETs, OPVs, memories, sensors).

Collaborations: G. Gu (UTK); D. Mandrus (UTK), G. Duscher (UTK), B. Hu (UTK); P. Hu (Haerbin Tech, China); J. Robinson (Penn State Univ.) D. Geohegan (ORNL), B. Sumpter (ORNL), V. Meunier (RPI), Y. Ma (ORNL), S. T. Pantelides (Vanderbilt Univ.), Y. Gogotsi (Drexel Univ.), P. Joshi (ORNL), C. H. Chen (NSRRC, Taiwan), H. Zhao (Univ. Kansas).

Graduate and Postdoctoral Advisors and Advisees:

Graduate Advisor: Profs. Daoben Zhu/Yunqi Liu (Institute of Chemistry, Chinese Academy of Sciences)

Postdoctoral Advisor: Dr. David B. Geohegan (Oak Ridge National Laboratory)

Graduate and Postdoctoral Advisees:

Postdoctoral:

Xufan Li, (Oak Ridge National Laboratory)

Bin Yang (Oak Ridge National Laboratory)

Kai Wang (Oak Ridge National Laboratory)

Ming Shao (currently working as "Thousand Young Talent Plan" professor at Beijing Jiaotong University)

Ming-Wei Lin, (currently working as Si Photonics Integration Engineer at SUNY Polytechnic Institute)

Guided and directed students:

William M Durant, May 10, 2010 – August 13, 2010, DOE HERE program, undergraduate student, Electrical & Computer Engineering, University of Alabama.

Kaylah Armstrong, Jun 2, 2014- August 8, 2014, undergraduate student, Talladega College, HBCU/MEI program.

Kun Lou, May, 2014 – August, 2014, PhD student, Bredesen Center Summer Internship.

Wan Deng, Mar 2011- May 2013, PhD student, co-advised with Prof Gong Gu at Department of Electrical Engineering and Computer Sciences at UTK.

Sanjib Das, Mar 2011- Jan 2016, PhD student, co-advised with Prof Gong Gu at Department of Electrical Engineering and Computer Sciences at UTK.

Akinola Oyedele, 2014-present, PhD student at Bredesen Center at UTK.

Funding grants: Department of Energy (BES, EERE); ORNL (LDRD).

1. DOE-BES Scientific User Facilities Division, Center for Nanophase Materials Sciences (2008-present).
2. Co-PI, DOE-BES Materials Science and Engineering Division, "Growth Mechanisms and Controlled Synthesis of Nanomaterials." (2013-2017).
3. PI, ORNL-LDRD, "Synthesis and Characterization of Novel Two-Dimensional Mesoscale Organic Nanomembranes", (2013-2015)
4. Co-PI, ORNL-LDRD, "Understanding dynamical structure-function evolution of electroactive molecules during thin film formation: dynamical control from nano- to mesoscale", (2013-2014)
5. Co-PI, ORNL-LDRD, "Untangling the role of boundaries, defects, and interfaces in 2D inorganic materials: a combined theoretical and experimental approach", (2014-2016)

6. Co-PI, DOE-EERE, "Novel photon management for thin-film photovoltaics". (2013-2015)
7. Co-PI, ORNL-LDRD, "Rational design of deuterated conjugated polymers with controlled spin-polarized electron transport". (2015-2017).

Recent Invited Talks and Contributed Conference Presentations

1. "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)
2. "Defect Engineering in Monolayer MoSe₂ through Controlled Synthesis and Doping", MRS Spring Meeting, Phoenix, AZ, April 16-21, 2017. (Invited talk)
3. "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.
4. "Epitaxial Growth and Optoelectronic Properties of 2D Materials", International Graphene Innovation Conference, Qingdao, China, September 22-24, 2016. (Invited talk).
5. "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)
6. "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)
7. "Isoelectronic Doping of MoSe₂ Monolayers for 2D Heterostructures", IUMRS-International Conference on Electronic Materials, Suntec, Singapore, July 4-8, 2016.
8. "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)
9. "Isoelectronic Doping of MoSe₂ Monolayers for 2D Heterostructures", Graphene and Beyond workshop, Penn State University, State College, PA, May 9-10, 2016. (Invited talk)
10. "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)
11. "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)
12. "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)
13. "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. (Invited seminar)
14. "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.
15. "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.
16. "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.
17. "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)
18. “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)
 19. “Revealing the Origin of High-Efficiency in Layer-by-Layer Processed Organometal Halide Perovskite Photovoltaics”, MRS spring conference, San Francisco, April 7-12, 2015.
 20. “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. (Invited seminar)
 21. “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)
 22. “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)
 23. “The isotopic effects deuteration on the optoelectronic properties of conducting polymers,” American Conference on Neutron Scattering, Knoxville, TN, USA, June 1-5, 2014.
 24. “Two-dimensional Chalcogenide Crystals: Synthesis, Characterization, and Optoelectronics”, Department of Materials Science and Engineering Seminar, University of Tennessee, Knoxville, March 7, 2014. (Invited seminar)
 25. “Substrate-mediated assembly and growth of organic semiconductor nanostructures,” The 5th International Conference on Nanoscience & Technology, Beijing, China, Sep. 5-7, 2013. (Invited talk)
 26. “Understanding the metal-directed growth of semiconducting organic nanocrystals,” Joint NSRC Workshop on Nanoparticle Science, November 5-6, 2012 Argonne National Laboratory.
 27. “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.
 28. “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.
 29. “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. (Invited talk)
 30. “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.
 31. “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.
 32. “One-Dimensional Electron-Transport in Self-Assembled Organic Nanowires,” 9th International Symposium on Functional π -Electron Systems, Atlanta, GA, Oct. 6, 2010.
 33. “Synthesis of Organic Semiconductor Nanowires for Solar Cells”, 3th Workshop on Sustainable Energy Future: Nanomaterials Enabled Photovoltaics, ORNL, Oak Ridge, TN, Sept. 22, 2010.

PUBLICATIONS (Over 100 articles in referred journals and books)

Full publication list available: [Kai Xiao](#)

Recent Book Chapters

1. B. Yang, D. Geoghegan, and K. Xiao, “Perovskite Materials: Solar Cell and Optoelectronic Applications”, Encyclopedia of Inorganic and Bioinorganic Chemistry (online), eibc2463 (2016).

- B. Yang, M. Shao, J. Keum, D. 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.
- D. B. Geohegan, A. A. Puzetky, 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.
- D. B. Geohegan, A. A. Puzetky, 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).
- 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).

Patents

- “Patterned Two-Dimensional Heterocrystals”, D. B. Geohegan, M-W. Lin, M. Mahjouri-Samani, A. Puzetky, C. M. Rouleau, K. Wang, K. Xiao, 201503565, DOE S-138,201.
- “Hybrid Perovskite Films”, D. B. Geohegan, O. E. Dyck, J. K. Keum, J. D. Poplawsky, K. Xiao, B. Yang, 20170098514.
- “Fabrication of Thin-Film Transistors Based on Aligned Carbon Nanotubes,” Y.Q. Liu, K. Xiao, P.A. Hu, G. Yu, X. B. Wang, D. B. Zhu, CN ZL 02145889.8, 2002.
- “Fabrication and Application of CN_x/C Nanotube Junctions,” Y. Q. Liu, P. A. Hu, K. Xiao, X. B. Wang, L. Fu, D. B. Zhu, CN ZL 02160815.6, 2002.
- “A Synthesis Method of Three-Dimensional Carbon Nanotube Alignments,” Y. Q. Liu, X. B. Wang, P. A. Hu, G. Yu, K. Xiao, and D. B. Zhu, CN ZL 02102542.8, 2002.
- “A New Method for the Fabrication of Nanotube-FET Devices Based on N-doped Carbon Nanotubes,” Y. Q. Liu, K. Xiao, P. A. Hu, G. Yu, L. Fu, D. B. Zhu, CN ZL 03108244, 2003.
- “Process for Preparing a CN_x/C Nanotube Diodes and Its Rectifying Properties,” Y. Q. Liu, K. Xiao, P. A. Hu, G. Yu, L. Fu, D.B. Zhu, CN ZL 03104280.5, 2003.
- “Fabrication Way and Application of 5,5'-bis-biphenyl-dithieno[3,2-b:2',3'-d]thiophene Compounds,” Y. Q. Liu, Y. Sun, Y. Ma, K. Xiao, G. Yu, D. Zhu, CN ZL 200410046350.8, 2004.
- “Fabrication Way of Field-Effect Transistors Controlled by Light Intensity,” Y. Q. Liu, K. Xiao, Y. Fu, G. Yu, Y. Luo, J. Zhai, L. Jiang, W. Hu and D. Zhu, CN ZL 200410101837.1, 2004.

Selected Refereed Journal Papers: (h-index 35, citations: 3868)

- Henry Yu, Nitant Gupta, Zhili Hu, Kai Wang, Bernadeta R Srijanto, Kai Xiao, David B Geohegan, Boris I Yakobson, *ACS Nano*, DOI: 10.1021/acsnano.7b0368 (2017).
- 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*, DOI: 10.1021/acs.nanolett.7b01047 (2017).
- Michael G Stanford; Pushpa R. Pudasaini; Elisabeth T. Gallmeier; Liangbo Liang; Nicholas Cross; Akinola Oyedele; Gerd Duscher; Masoud Mahjouri-Samani; Kai Wang; Kai Xiao; David B. Geohegan; Alex Belianinov; Bobby G. Sumpter; Philip D. Rack, *Advanced Functional Materials*, 10.1002/adfm.201702829 (2017).
- 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).

5. 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).
6. 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).
7. 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 Res.* doi:10.1007/s12274-017-1681-5 (2017).
8. Pushpa Raj Pudasaini, Michael G Stanford, Akinola Oyedele, Anthony Wong, Anna Hofmann, Dayrl Briggs, Kai Xiao, David G Mandrus, Thomas Z Ward, Philip D Rack, *Nanotechnology*, doi.org/10.1088/1361-6528/aa8081(2017).
9. 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).
10. 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).
11. 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*, 2DM-101002 (2016).
12. 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).
13. X. Li, A. A. Puztzky, 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*, DOI:10.1002/adfm.201603850 (2016)
14. X. Li, M.-W. Lin, L. Basile, S. M. Hus, A. A. Puztzky, 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).
15. X. Li, M.-W. Lin, J. Lin, B. Huang, A. A. Puztzky, 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).
16. 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).
17. 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)
18. 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).
19. X. Li, M.-W. Lin, A. A. Puztzky, 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”)
20. M.-W. Lin, I. Kravchenko, J. Fowlkes, X. Li, A. Puzos, C. Rouleau, D. Geohegan, **K. Xiao***, “Thickness Dependent Charge Transport in Few-Layer MoS₂ Field-Effect Transistors”, *Nanotechnology*, 27, 165203 (2016).
 21. M. Lin, H. L Zhuang, J. Yan, T. Z. Ward, A. A Puzos, 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).
 22. 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).
 23. 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).
 24. 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. Puzos, **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 MoSe_{2-x} Crystals”, *Nano Lett.*, 16, 5213 (2016).
 25. K. Wang, B. Huang, M. Tian, F. Ceballos, M.-W. Lin, M. Mahjouri-Samani, A. Boulesbaa, A. A. Puzos, 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).
 26. 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).
 27. 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).
 28. 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).
 29. A. A. Puzos, 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).
 30. 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).
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