Selected Representative Publications

October 2021

As of October 2021, Professor Luo has authored and co-authored >165 articles (counting >90 articles as a corresponding author) in high-quality peer-reviewed journals, including *Acta Materialia* (19), *Scripta Materialia* (18), *Science* (4), *Nature* (1), *Nature Communications* (3), *Nature Catalysis* (1), *Science Advances* (2), *Materials Today* (3), *Physical Review Letters* (2), *Materials Horizons* (2), *npj Computational Materials* (1), *Nano Letters* (2), *Energy Storage Materials* (1), *Journal of the European Ceramics Society* (10), *Journal of the American Ceramics Society* (6), *Applied Physics Letters* (7), *ACS Applied Materials & Interfaces* (4), *Journal of Power Sources* (4), *Advanced Materials* (2), *Advanced Functional Materials* (1), *Annual Review of Materials Research* (1), *Critical Review in Solid State and Materials Science* (1), *Current Opinion in Solid State and Materials Science* (3), *Review of Modern Physics* (1), and *Journal of Materials Science* (3).

Sixty (60) selected representative publications in several areas are listed below.

(**1a**) Selected Articles on Computing Grain Boundary "Phase" (Complexion) Diagrams:

1. C. Hu and J. Luo, "Data-Driven Prediction of Grain Boundary Segregation and Disordering in High-Entropy Alloys in a 5D Space," *Materials Horizons*, DOI: 10.1039/D1MH01204E
2. C Hu, Y Li, Z Yu, J Luo, "Computing Grain Boundary Diagrams of Thermodynamic and Mechanical Properties," *npj Computational Materials,* 7, 159 (2021).
3. N. Zhou, C. Hu, J. Luo, "Grain Boundary Segregation Transitions and Critical Phenomena in Binary Regular Solutions: A Systematics of Complexion Diagrams with Universal Characters," *Acta Materialia*, 221, 117375 (2021).
4. C. Hu, Y. Zuo, C. Chen, S. Ping Ong, J. Luo*, "Genetic Algorithm-Guided Deep Learning of Grain Boundary Diagrams: Addressing the Challenge of Five Degrees of Freedom," *Materials Today*, 38, 49-57 (2020). (**Predicting Grain Boundary Properties in a 7D Space**)
5. S. Yang, N. Zhou, H. Zheng, S. P. Ong, J. Luo*, "First-Order Interfacial Transformations with a Critical Point: Breaking the Symmetry at a Symmetric Tilt Grain Boundary," *Physical Review Letters*, 120, 085702 (2018) (**The First Grain Boundary "Phase" Diagram from Atomistic Simulations**)
6. N. Zhou, Z. Yu, Y. Zhang, M.P. Harmer, J. Luo*, "Calculation and Validation of a Grain Boundary Complexion Diagram for Bi-doped Ni," *Scripta Materialia,* 130, 165-169 (2017).
7. N. Zhou, J. Luo*, "Developing Grain Boundary Diagrams for Multicomponent Alloys," *Acta Materialia*, 91, 202-16 (2015).
8. X. Shi, J. Luo*, "Developing Grain Boundary Diagrams as a Materials Science Tool: A Case Study of Nickel-doped Molybdenum," *Physical Review B*, 84, 014105 (2011). (**An Editors' Suggestion**: ~4-8% articles in *Phys. Rev. B* "that the editors and referees find of particular interest, importance, or clarity")

9. X. Shi, J. Luo*, "Decreasing the Grain Boundary Diffusivity in Binary Alloys with Increasing Temperature," *Physical Review Letters*, 105, 236102 (2010)

10. J. Luo*, X. Shi, "Grain Boundary Disordering in Binary Alloys," *Applied Physics Letters*, 92, 101901 (2008). (**The First Paper to Compute Grain Boundray λ Diagrams from Thermodynamic Models**)

(**1b**) Selected Articles on Grain Boundary Embrittlement and Other Discoveries of Complexions:

11. T. Hu, S. Yang, N. Zhou, Y. Zhang, J. Luo*, "Role of Disordered Bipolar Complexions on the Sulfur Embrittlement of Nickel General Grain Boundaries," *Nature Communications*, 9, 2764 (2018). UCSD News; MRS News Article; DoD Basic Research on Twitter (**Uncovering the Atomic-Level Grain Boundary Embrittlement Mechanism in Ni-S, a System of Great Technological Importance**)

12. J. Luo*, H. Cheng, K. M. Asl, C. J. Kiely, M. P. Harmer*, "The Role of a Bilayer Interfacial Phase on Liquid Metal Embrittlement," *Science*, 333, 1730-33 (2011) (**Uncovering the Mysterious Atomic-Level Liquid Metal Embrittlement Mechanism in Ni-Bi**)

13. Z. Yu, P. R. Cantwell, Q. Gao, D. Yin, Y. Zhang, N. Zhou, G. S. Rohrer, M. Widom, J. Luo*, M. P. Harmer*, "Segregation-Induced Ordered Superstructures at General Grain Boundaries in a Ni-Bi Alloy," *Science*, 358, 97–101 (2017) UCSD News Release (**Reconstruction at General Boundaries**)

14. C. Yang, C. Hu, C. Xiang, H. Nie, X. Gu, L. Xie, J. He, W. Zhang, Z. Yu*, J. Luo*, "Interfacial Superstructures and Chemical Bonding Transitions at Metal-Ceramic Interfaces," *Science Advances*, 7, eabf6667 (2021) (**Metal-Ceramic Interfaces: How does a metal transit to a ceramic?**)

15. Z. Luo, C. Hu, L. Xie, H. Nie, C. Xiang, X. Gu, J. He, W. Zhang*, Z. Yu*, J. Luo*, "A Highly Asymmetric Interfacial Superstructure in WC: Expanding the Classic Grain Boundary Segregation and New Complexion Theories," *Materials Horizons*, 7, 173-180 (2020). (**Asymmetrical Boundaries**)

16. X. Shi and J. Luo*, "Grain Boundary Wetting and Prewetting in Ni-doped Mo," *Applied Physics Letters*, 94, 251908 (2009).

17. J. Luo*, V. K. Gupta, D.H. Yoon, H. M. Meyer III, "Segregation-Induced Grain Boundary Premelting in Nickel-doped Tungsten," *Applied Physics Letters*, 87, 231902 (2005). (**Discovery of Premelting Like Amorphous Intergranular Films in Metals – The First Direct HRTEM Evidence**)

(**1c**) Novel Thermodynamics Based Interfacial Engineering of Materials for Energy Applications:

18. J. Luo, "Let thermodynamics Do the Interfacial Engineering of Batteries and Solid Electrolytes," *Energy Storage Materials*, 21, 50-60 (2019). (**Invited Review**)

19. W. Liu, W. Pan*, J. Luo*, A. Godfrey, G. Ou, H. Wu, and W. Zhang, "Suppressed phase transition and giant ionic conductivity in $La_2Mo_2O_9$ nanowires," *Nature Communications*, 6,

8354 (2015).

20. M. Samiee, and J. Luo, "Pseudocapacitive Properties of Two-Dimensional Surface Vanadia Phases Formed Spontaneously on Titania," *ACS Applied Materials & Interfaces*, 8, 12871–12880 (2016).
21. J. Huang and J. Luo, "A Facile and Generic Method to Improve Cathode Materials for Lithium-ion batteries via Utilizing Nanoscale Surface Amorphous Films of Self-Regulating Thickness," *Physical Chemistry Chemical Physics*, 16, 7786-7798 (2014).
22. A. Kayyar, H. Qian, and J. Luo, "Surface Adsorption and Disordering in $LiFePO_4$ Based Battery Cathodes," *Applied Physics Letters*, 95, 221905 (2009).
23. J. Luo and Y.-M. Chiang, "Wetting and Prewetting on Ceramic Surfaces" *Annual Review of Materials Research*, 38, 227-249 (2008). (**Invited Review**)

(**2a**) Uncovering the Mysterious Mechanisms of Solid-State Activated Sintering:

24. J. Nie, J. M. Chan, M. Qin, N. Zhou, and J. Luo*, "Liquid-Like Grain Boundary Complexion and Sub-Eutectic Activated Sintering in CuO-Doped TiO_2," *Acta Materialia*, 130, 329-338 (2017).
25. J. Luo*, "Developing Interfacial Phase Diagrams for Applications in Activated Sintering and Beyond: Current Status and Future Directions," *Journal of the American Ceramic Society*, 95, 2358-71 (2012). (**Cover & Lead Article**; also featured in *Ceramics Tech Today* and *American Ceramic Society Bulletin*, 91 (8), p. 17-18.)
26. J. Luo*, "Liquid-Like Interface Complexion: from Activated Sintering to Grain Boundary Diagrams," *Current Opinion in Solid State & Materials Science*, 12, 81-88 (2008). (**Invited Perspective**)
27. V. K. Gupta, D. H. Yoon, H. M. Meyer III, and J. Luo*, "Thin Intergranular Films and Solid-State Activated Sintering in Nickel-Doped Tungsten," *Acta Materialia*, 55, 3131-3142 (2007).
28. J. Luo, H. Wang, and Y. -M. Chiang, "Origin of Solid State Activated Sintering in Bi_2O_3-Doped ZnO," *Journal of the American Ceramic Society*, 82, 916-20 (1999).

(**2b**) Flash Sintering and Ultrafast Sintering without Electric Fields:

29. C. Wang, W. Ping, Q. Bai, H. Cui, R. Hensleigh, R. Wang, A.H. Brozena, Z. Xu, J. Dai, Y. Pei, C. Zheng, G. Pastel, J. Gao, X. Wang, H. Wang, J.-C. Zhao, B. Yang, X. Zheng*, J. Luo*, Y. Mo*, B. Dunn, L. Hu*, "A General Method to Synthesize and Sinter Bulk Ceramics in Seconds," *Science*, 368, 521-26 (2020). **Cover Article for the May 1, 2020 Issue of *Science*** *Ceramics Tech Today* News
30. J. Luo*, "The Scientific Questions and Technological Opportunities of Flash Sintering: From a Case Study of ZnO to Other Ceramics", *Scripta Materialia*, 146, 260-66(2018). (**Invited Viewpoint for Flash Sintering**)
31. Y. Zhang, J.Y. Nie, J.M. Chan, J. Luo*, "Probing the Densification Mechanisms During Flash Sintering of ZnO," *Acta Materialia*, 125, 465 (2017). (**Uncovering the Mechanisms of Flash Sintering + The First Report of Rapid Thermal Annealing with IR Heating to Sinter**

ZnO in Seconds without an Electric Field)

32. Y. Zhang, J.-I. Jung, and J. Luo*, "Thermal Runaway, Flash Sintering and Asymmetrical Microstructural Development of ZnO and ZnO–Bi_2O_3 under Direct Currents," *Acta Materialia*, 94, 87-100 (2015). (**Uncovering the Mechanisms of Flash Sintering: The First to Reveal That "Flash" Starts as a Thermal Runaway**, along with an Independent Report from Oxford Submitted 10 Days Later)
33. J. Nie, Y. Zhang, J.M. Chan, S. Jiang, R. Huang, and J. Luo*, "Two-Step Flash Sintering of ZnO: Fast Densification with Suppressed Grain Growth," *Scripta Materialia*, 141, 6-9 (2017). (**A New Innovative Flash Sintering Method**)
34. J. Nie, Y. Zhang, J.M. Chan, R. Huang, and J. Luo*, "Water-Assisted Flash Sintering: Flashing ZnO at Room Temperature to Achieve ~ 98% Density in Seconds," *Scripta Materialia*, 142, 79-82 (2018). (**A New Innovative Flash Sintering Method**)

(**2c**) A New Discovery – Electric Field Effects on Microstructural Evolution:

35. J. Nie, C. Hu, Q. Yan, J. Luo*, "Discovery of Electrochemically Induced Grain Boundary Transitions," *Nature Communications*, 12, 2374 (2021).

(**3**) Selected Articles on Pushing the Boundary of High-Entropy Materials:

36. J. Gild, Y. Zhang, T. Harrington, S. Jiang, T. Hu, M. C. Quinn, W. M. Mellor, N. Zhou, K. Vecchio, and J. Luo*, "High-Entropy Metal Diborides: A New Class of High-Entropy Materials and a New Type of Ultrahigh Temperature Ceramics," *Scientific Reports*, 6, 37946 (2016). (**The First Report of High-Entropy Borides/UHTCs** and **the Second Bulk High-Entropy Ceramics Fabricated**) Cited *374 times* as of 10/25/2021.
37. S. Jiang, T. Hu, J. Gild, N. Zhou, J. Nie, M. Qin, T. Harrington, K. Vecchio, and J. Luo*, "A New Class of High-Entropy Perovskite Oxides," *Scripta Materialia*, 142, 116-20 (2018). (**The First Report of High-Entropy Perovskites**) Cited *290 times* as of 10/25/2021; **the most cited article in *Scripta Materialia*** since 2018.
38. J. Gild, M. Samiee, J. L. Braun, T. Harrington, H. Vega, P. E. Hopkins, K. Vecchio, and J. Luo*, "High-Entropy Fluorite Oxides," *Journal of the European Ceramic Society*, 38, 3578-84 (2018). (**The First Study of YSZ-Like High-Entropy Oxides for TBCs**) Cited *198 times* as of 10/25/2021; the second most cited article (and the most cited research article) in *Journal of the European Ceramic Society* since 2018.
39. J. Gild, J. Braun, K. Kaufmann, E. Marin, T. Harrington, P. Hopkins, K. Vecchio, J. Luo*,"A high-entropy silicide: $(Mo_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2}W_{0.2})Si_2$," *Journal of Materiomics*, 5, 337-43 (2019). (**One of Two First Simultaneous Reports of High-Entropy Silicides**) Cited *99 times* as of 10/25/2021.
40. M. Qin, Q. Yan, H. Wang, C. Hu, K.S. Vecchio, J. Luo*, "High-Entropy Monoborides: Towards Superhard Materials," *Scripta Materialia*, 189, 101-105 (2020). (**The First Report of High-Entropy Monoborides** and **the First Superhard High-Entropy Materials**)
41. M. Qin, J. Gild, C. Hu, H. Wang, M. S. B. Hoque, J. L. Braun, T.J. Harrington, P. E. Hopkins, S. Vecchio, J. Luo*, "Dual-Phase High-Entropy Ultrahigh Temperature Ceramics," *Journal*

of the European Ceramic Society, 40, 5037-5050 (2020). (**The First Study of Dual-Phase High-Entropy Ceramics** and **Discovery of an Important Thermodynamic Relation**)

42. J. Wright, Q. Wang, C. Huang, A. Nieto, R. Chen, J. Luo*, "From High-Entropy Ceramics to Compositionally-Complex Ceramics: A Case Study of Fluorite Oxides," *Journal of the European Ceramic Society*, 40, 2120-29 (2020). (**The First Publication to Propose to Extend "High-Entropy Ceramics (HECs)" to "Compositionally-Complex Ceramics (CCCs)"**)
43. A.J. Wright, J. Luo*, "A Step Forward from High-Entropy Ceramics to Compositionally Complex Ceramics: A New Perspective," *Journal of Materials Science*, 55, 9812-9827 (2020). (**Invited Perspective for the 1000th Issue,** inadvertently published in the 999th Issue); (**Further Elaboration of the New Concepts Underpinning "Compositionally-Complex Ceramics (CCCs)"**)
44. N. Zhou, S. Jiang, T. Huang, M. Qin, T. Hu, and J. Luo*, "Single-Phase High-Entropy Intermetallic Compounds (HEICs): Bridging High-Entropy Alloys and Ceramics," *Science Bulletin*, 64, 856-64 (2019). (**The First Study of Single-Phase High-Entropy Intermetallic Compounds to Bridge High-Entropy Alloys and Ceramics**)
45. J. Wright, Q. Wang, S. T. Ko, K. M. Chung, R. Chen, J. Luo*, "Size Disorder as a Descriptor for Predicting Reduced Thermal Conductivity in Medium- and High-Entropy Pyrochlore Oxides," *Scripta Materialia*, 181, 76-81 (2020). (**New Insight on Reduced Thermal Conductivities in HECs/CCCs**)
46. M. Qin, Q. Yan, Y. Liu, J. Luo, "A New Class of High-Entropy M_3B_4 Borides," *Journal of Advanced Ceramics* 10, 166-172 (2021). (**The First Report of High-Entropy M_3B_4 Borides**)
47. M. Qin, Q. Yan, H. Wang, K. S. Vecchio, J. Luo, "High-Entropy Rare Earth Tetraborides" *Journal of the European Ceramic Society*, 41, 2968-73 (2021). (**The First Report of High-Entropy Tetraborides**)
48. A. J. Wright, Q. Wang, C. Hu, Y. T. Yeh, R. Chen, J. Luo, "Single-Phase Duodenary High-Entropy Fluorite/Pyrochlore Oxides with an Order-Disorder Transition," *Acta Materialia,* 211, 116858 (2021). (**Discovery of Order-Disorder Transitions in Duodenary High-Entropy Oxides**)
49. J. Gild, K. Kaufmann, K. Vecchio, J. Luo*, "Reactive Flash Spark Plasma Sintering of High-Entropy Ultrahigh Temperature Ceramics," *Scripta Materialia*, 170, 106-10(2019). (**Ultrafast Synthesis and Densification of $(Zr_{0.2}Hf_{0.2}Ti_{0.2}Ta_{0.2}Nb_{0.2})B_2$ to >99% Relative Density in 120 s**)
50. N. Zhou, T. Hu, J. Huang, J. Luo*, "Stabilization of Nanocrystalline Alloys at High Temperatures via Utilizing High-Entropy Grain Boundary Complexions," *Scripta Materialia*, 124, 160-163 (2016). (**Original Paper of Using High-Entropy Grain Boundaries to Stabilize Nanoalloys at High *T*'s**)

<u>Five Selected Invited Reviews or Perspectives</u>:

51. J. Luo, "Stabilization of Nanoscale Quasi-Liquid Interfacial Films in Inorganic Materials: A Review and Critical Assessment"**,** *Critical Reviews in Solid State and Materials Sciences*, 32,

67-109 (2007). (**Invited** and **Cover Article**)

52. P. R. Cantwell, M. Tang, S. J. Dillon, J. Luo, G. S. Rohrer, M. P. Harmer, "Overview No. 152: Grain Boundary Complexions," *Acta Materialia*, 62, 1-48 (2014). (**Invited Overview**)
53. N. Zhou, T. Hu, J. Luo*****, "Grain Boundary Complexions in Multicomponent Alloys: Challenges and Opportunities," *Current Opinion in Solid State and Materials Science*, 20, 268-277 (2016). (**Invited**)
54. Q. Yan, G. Whang, Z. Wei, S.-T. Ko, P. Sautet, S. H. Tolbert, B. Dunn, J. Luo*****, "A Perspective on Interfacial Engineering of Lithium Metal Anodes and Beyond," *Applied Physics Letters*, 117, 080504 (2020) (**Invited Perspective** and **Editor's Pick**)
55. J. Luo*****, "Interfacial Engineering of Solid Electrolytes," *Journal of Materiomics*, 1, 22-32 (2015). (**Invited for the launching Issue**).

Five Selected Research Articles in Other Technological Areas:

56. Y Zuo, M Qin, C Chen, W Ye, X Li, J Luo*****, SP Ong*****, "Accelerating Materials Discovery with Bayesian Optimization and Graph Deep Learning," *Materials Today*, 51, 126-135 (2021)
57. H. Gao, Y. Hu, Y. Xuan, J. Li, Y. Yang, R.V. Martinez, C. Li, J. Luo, M. Qi, G.J. Cheng, "Large Scale Nanoshaping of Ultrasmooth 3D Crystalline Metallic Structures," *Science*, 346, 1352-1356 (2014).
58. Y. Lei, Y. Chen, R. Zhang, Y. Li, Q. Yan, S. Lee, Y. Yu, H. Tsai, W. Choi, K. Wang, Y. Luo, Y. Gu, X. Zheng, C. Wang, C. Wang, H. Hu, Y. Li, B. Qi, M. Lin, Z. Zhang, S.A. Dayeh, M. Pharr, D.P. Fenning, Y.-H. Lo, J. Luo, K. Yang, J. Yoo, W. Nie, S. Xu, "A Fabrication Process for Flexible Single-Crystal Perovskite Devices," *Nature*, 583, 790-795 (2020).
59. H. Chen, G. Zhang, Z. Wei, K. M. Cooke, and J. Luo*****, "Layer-by-Layer Assembly of Sol-Gel Oxide "Glued" Montmorillonite-Zirconia Multilayers," *Journal of Materials Chemistry*, 20, 4925-4936 (2010).
60. J. Luo, "Modeling Dissimilar Optical Fiber Splices with Substantial Diffusion," *IEEE/OSA Journal of Lightwave Technology*, 25, 3575-3579 (2007) (**Selected Industrial Research**)