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❖ Publications: (underlined are undergraduate co-authors, * are Sparks Group members)

Submitted

1. Christopher M. Collins[ł], Hasan M. Sayeed*[ł], George R. Darling, John B. Claridge, **Taylor D. Sparks**, and Matthew J. Rosseinsky "Integration of generative machine learning with the heuristic crystal structure prediction code FUSE" *under review*.
2. Sterling G. Baird*, Jeet N. Parik*, and **Taylor D. Sparks** "Materials Science Optimization Benchmark Dataset for High-dimensional, Multi-objective, Multi-fidelity Optimization of CrabNet Hyperparameters" *under review*.
3. Marcus E. Parry*, Cheng Sun, Boopathy Kombaiah, Wen Jiang, Xiaofei Pu, David Frazer, Seongtae Kwon, Jeffery A. Aguiar, and **Taylor D. Sparks "**Microstructure, mechanical properties, and irradiation response of AlxCrFeNi(Cu,Mn) multi-principal element alloys" *under review*.
4. Pooya Elahi*, Jude A. Horsley*, and **Taylor D. Sparks** "Synthesis and Electrochemical Study of Multi-Phase, Multi-Species Ion Conductor Sodium β''-Alumina (BASE) + 20SDC Using a Vapor-Phase Process" *under review*.

Accepted or published

1. Stanley Lo, Nessa Carson, Sterling G. Baird*, Ian Foster, Joshua Schrier, BenBlaiszik, Andres Aguilar-Granda, Sergei V. Kalinin, Benji Maruyama, Maria Politi, Helen Tran, **Taylor D. Sparks**, and Alan Aspuru-Guzik "Review of Low-cost Self-driving Laboratories in Chemistry and Materials Science: The "Frugal Twin" Concept" *Digital Discovery, accepted February 13 2024.* [DOI]
2. Hasan M. Sayeed*, Trupti Mohanty*, and **Taylor D. Sparks** "Annotating Materials Science Text: A Semi-Automated Approach for Crafting Outputs with Gemini Pro" *accepted to Integrating Materials and Manufacturing Innovation on April 10th 2024.*
3. Federico Ottomano, Giovanni De Felice, Vladimir Gusev, and **Taylor D. Sparks** "Not as simple as we thought: A rigorous examination of data aggregation in materials informatics" *Digital Discovery*, **3**, 337-346 (2024). [DOI]
4. Hasan M. Sayeed*, Wade Smallwood*, Sterling G. Baird, and **Taylor D. Sparks** "NLP meets Materials Science: Quantifying the presentation of materials data in scientific literature" *Matter*, **7** [3], 723-727 (2024). [DOI]
5. Michael Alverson*, Sterling G. Baird*, Ryan Murdock*, (Enoch) Sin-Hang Ho, Jeremy Johnson, and **Taylor D. Sparks** "Generative adversarial networks and diffusion models in material discovery" *Digital Discovery*, **3**, 62-80 (2024). [DOI]
6. Travis Allen*, Jake Graser*, Ramsey Issa*, and **Taylor D. Sparks** "Machine learning predictions of low thermal conductivity: comparing TaVO5 and GdTaO4" *Advances in Applied Ceramics on October 19 2023.* [DOI]
7. **Taylor D. Sparks** "Tales from Sabbatical III: Coming Home" *Matter*, **6** [12], 4111-4115 (2023). [DOI]
8. Shadi Al Khateeb*, Brian T. Bennett, James P. Beck, Sujee Jeyapalina, **Taylor D. Sparks** "Crystallinity evolution of spray pyrolyzed fluorapatite thin film by post-deposition treatment" *Thin Solid Films*, **784**, 140082 (2023). [DOI]
9. Jason R. Hall* and **Taylor D. Sparks** "A Case Study of β-Variational Auto-Encoder Disentanglement with Different Input Distributions for Computational Multi-modal Particle Packing" *Integrating Materials and Manufacturing Innovation*, **12**, 267-275 (2023). [DOI]
10. Sterling G. Baird*, Ramsey Issa*, and **Taylor D. Sparks** "Materials Science Optimization Benchmark Dataset for Multi-fidelity Hard-sphere Packing Simulations" *Data in Brief*, **50**, 109487 (2023). [DOI]

11. Colton C. Seegmiller*, Sterling G. Baird*, Hasan M. Sayeed*, and **Taylor D. Sparks** "Discovering Chemically Novel, High-Temperature Superconductors" *Computational Materials Science*, 228, 112358 (2023). [DOI]
12. Trupti Mohanty*, K.S. Ravi Chandran, **Taylor D. Sparks** "Machine learning guided optimal composition selection of niobium alloys for high temperature applications" *APL Machine Learning*, **1**, *036102* (2023). [DOI]
13. Kaitlin Tyler, Enze Chen, Bryce Meredig, and **Taylor D. Sparks** "Artificial intelligence in materials education: A roundtable discussion" *JOM*, **75**, 2083-2085 (2023). [DOI]
14. Shadi Al Khateeb*, Brian T. Bennett, Sujee Jeyapalina, James P. Beck, **Taylor D. Sparks** "Morphological evolution effect on the bio-performance of spray pyrolysis-based synthesis of fluorapatite thin films" *JOM*, **75**, 3332-3344 (2023). [DOI]
15. Sterling G. Baird* and **Taylor D. Sparks** "Building a "Hello World" for Self-driving Labs: The Closed-loop Spectroscopy Lab Light-mixing Demo (CLSLab:Light)" *STAR Protocols*, **4**, 102329 *(2023)*. [DOI]
16. Erick A. Lawrence, Matthew Davenport, Reshma Devi, Zijian Cai, Maxim Avdeev, Jonathan R. Belnap, Husain Alnaser*, Alice Ho, **Taylor D. Sparks**, Gopalakrishnan Sai Gautam, Jared Allred, Huiwen Ji "Reversible Electrochemical Lithium Cycling in a Vanadium(IV) and Niobium(V)-based Wadsley-Roth Phase" *Chemistry of Materials*, **35** [9], 3470-3483 (2023). [DOI]
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18. Husain F. Alnaser* and **Taylor D. Sparks** "BSTS Synthesis Guided by CALPHAD Approach for Phase Equilibria and Process Optimization" *Scientific Reports*, **13**, 3944 (2023). [DOI]
19. Shadi Al Khateeb*, Brian T. Bennett, Sujee Jeyapalina, James P. Beck, **Taylor D. Sparks** "Exploration of fluorapatite bio-ceramic thin film deposition by ultrasonic spray pyrolysis" *Journal of Materials Research*, **38**, 2287-2301 (2023). [DOI]
20. **Taylor D. Sparks** "Tales from Sabbatical II: During your stay" *Matter*, **6** [3], 648-652 (2023). [DOI]
21. Husain F. Alnaser*, Stacey J. Smith, and **Taylor D. Sparks** "Structural Investigations of the Bi2–xSbxTe3–ySey Topological Insulator" *Journal of Solid State Chemistry*, **320**, 123868 (2023). [DOI]
22. Pooya Elahi*, Elizabeth Winterholler*, Jude Horsley*, and **Taylor D. Sparks** "The Influence of Sintering Condition on Microstructure, Phase Composition, and Electrochemical Performance of the Scandia- Ceria- Co- Doped Zirconia for SOFCs," *Science of Sintering*, **55**, 237-258 (2023). [DOI]
23. Sterling G. Baird* and **Taylor D. Sparks** "What is a minimal working example for a materials acceleration platform?" *Matter*, **5** [12]4170-4178 (2022). [DOI]
24. Pooya Elahi*, Jude A. Horsley*, and **Taylor D. Sparks** "Electrochemical and Degradation Studies on One-Dimensional Tunneled Sodium Zirconogallate + Yttria-Stabilized Zirconia Composite, Mixed Sodium and Oxygen Ion Conductor" *Journal of the Electrochemical Society*, **169** [11] 114502 (2022). [DOI]
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27. Sterling G. Baird*, Kevin M. Jablonka, Michael D. Alverson*, Hasan M. Sayeed*, Mohammed Faris Kahn*, Colton Seegmiller*, Berend Smit, and **Taylor D. Sparks** "xtal2png: A Python package for representing crystal structure as PNG files" *Journal of Open Source Software*, **7** [76], 4528 (2022). [DOI]
28. Richard Edwards, Isaac Krieger*, Mark P. Halling*, Shelley Minteer, **Taylor D. Sparks**, and David Schurig "Additive-Manufactured, Highly-Conductive Metasurfaces, with Application Enabling Secondary Properties, for Microwave Waveguide Components" *IEEE Access*, **10**, 58921-58929 (2022). [DOI]
29. Sterling G. Baird*, Marianne Liu*, and **Taylor D. Sparks** "High-dimensional Bayesian Optimization of Hyperparameters for an Attention-based Network to Predict Materials Property: a Case Study on CrabNet using Ax and SAASBO", *Computational Materials Science,* **211**, 111505 (2022). [DOI]

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31. Raju Baral, Jacob Christensen, Parker Hamilton, Feng Ye, Milinda Abeykoon, Karine Chesnel, **Taylor D. Sparks**, Rosa Ward*, Jiaqiang Yan, Michael E. Manley, Raphael P. Hermann, and Benjamin A. Frandsen "Real-space visualization of short-range antiferromagnetic correlations in MnTe" *Matter,* **5** [6], 1853-1864 (2022). [DOI]
32. Marcus E. Parry*, Samantha Couper, Jackson Hendry*, Aria Mansouri Tehrani, Anton O. Oliynyk, Jakoah Brgoch, Lowell Miyagi, and **Taylor D. Sparks** "Trends in bulk compressibility of $Mo_{2-x}W_xBC$ solid solutions" *Chemistry of Materials*, **34** [6], 2569-2575 (2022). [DOI]
33. Sterling G. Baird and **Taylor D. Sparks** "High-throughput calculation of atomic planar density for compounds" *Journal of Applied Crystallography,* **55**, 380-385 (2022). [DOI]
34. Maria-Magdalena Titirici, Sterling G. Baird*, **Taylor D. Sparks**, Shirley M. Yang, Agi Brandt-Talbot, Omid Hosseinaei, David Paul Harper, Richard Parker, Silvia Vignolini, Lars Berglund, Yuanyuan Li, Huai-Ling Gao, Li-Bo Mao, Shuhong Yu, Noel Díez, Guillermo Alvarez.ferrero, Marta Sevilla Solis, Petra Szilagyi, Connor Stubbs, Joshua Worch, Yunping Huang, Christine Luscombe, Koon-yang Lee, Hui Luo, Jim Platts, Devendra Tiwari, Dmitry Kovalevskiy, David Fermin, Heather Au, Hande Alptekin, Maria Crespo Ribadeneyra, Valeska Ting, Tim-Patrick Fellinger, Jesus Barrio-hermida, Olivia Westhead, Claudie Roy, Ifan Stephens, Sabina Alexandra Nicolae, Saurav Sarma, Rose Oates, Chen Gang Wang, Zibiao Li, Xian Jun Loh, Rupert J Myers, Niko Heeren, Alice Grégoire, Clément Périssé, Xiaoying Zhao, Yael Vodovotz, Becky Earley, Goran Finnveden, Anna Björklund, Gavin Harper, Allan Walton, and Paul A Anderson "The sustainable materials roadmap" *JPhys Materials*, **5**, 032001 (2022). [DOI]
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37. **Taylor D. Sparks** "Inaugural Congress to Focus on Artificial Intelligence" *JOM*, **73**, 3679-3680 (2021). [DOI]
38. Andrew Falkowski*, Steven K. Kauwe*, and **Taylor D. Sparks** "Optimizing fractional compositions to achieve extraordinary properties" *Integrating Materials and Manufacturing Innovation*, **10**, 689-695 (2021). [DOI]
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40. Jason R. Hall*, Steven K. Kauwe*, and **Taylor D. Sparks** "Sequential Machine Learning Applications of Particle Packing with Large Size Variations" *Integrating Materials and Manufacturing Innovation*, **10**, 559-567 (2021). [DOI]
41. Ashley N Henderson*, Steven K Kauwe*, and **Taylor D. Sparks** "Benchmark datasets incorporating diverse tasks, sample sizes, material systems, and data heterogeneity for materials informatics" *Data in Brief*, **37**, 107262 (2021). [DOI]
42. Akira Nagaoka, Kenji Yoshino, Taizo Masuda, **Taylor D. Sparks**, Michael A. Scarpulla, and Kensuke Nishioka "Environmentally friendly thermoelectric sulfide Cu2ZnSnS4 single crystals with dimensionless figure of merit achieving 1.6" *Journal of Materials Chemistry A*, **9**, 15595-15604 (2021). [DOI]
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44. **Taylor D. Sparks** and Debanshu Banerjee* "Materials Informatics and Polymer Science: Pushing the Frontiers of our Understanding" *Matter*, **4** [5], 1454-1456 (2021). [DOI]
45. Logan G. Kiefer*, Christian J. Robert*, and **Taylor D. Sparks** "Lifetime of electrochromic optical transition cycling of ethyl viologen diperchlorate-based electrochromic devices" *SN Applied Sciences,* **3**, 554 (2021). [DOI]

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48. Ryan Murdock*, Steven K. Kauwe*, Anthony Yu-Tang Wang*, and **Taylor D. Sparks** "Is domain knowledge necessary for machine learning materials properties?" *Integrating Materials and Manufacturing Innovation,* **9**, 221-227 (2020). [DOI]
49. (invited) Amber Barron* and **Taylor D. Sparks** "Commercial Marine-degradable Polymers for Flexible Packaging" *iScience,* **23**, 101353, (2020). [DOI]
50. Steven K. Kauwe*, Taylor M. Welker, and **Taylor D. Sparks** "Extracting Knowledge from DFT: Experimental Band Gap Predictions Through Ensemble Learning" *Integrating Materials and Manufacturing Innovation,* **9**, 213-220, (2020). [DOI]
51. (invited) Anthony Yu-Tang Wang, Ryan J. Murdock*, Steven K. Kauwe*, Anton O. Oliynyk, Aleksander Gurlo, Jakoah Brgoch, Kristin A. Persson, and **Taylor D. Sparks** "Machine Learning for Materials Scientists: An introductory guide towards best practices" *Chemistry of Materials*, **32**, [12], 4954–4965 (2020). [DOI]
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57. (invited) Steven K. Kauwe*, Jake Graser*, Ryan Murdock*, and **Taylor D. Sparks** "Can machine learning find extraordinary materials?" *Computational Material Science*, **174**, 109498 (2020). [DOI]
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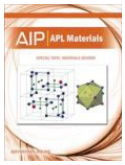

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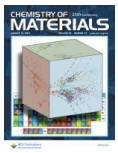

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3. Amber N. Barron, Ashlea Patterson, and **Taylor D. Sparks** "Hydrogel synthesis" JoVE Science Education Database. Inactive Collection. JoVE, Cambridge, MA, (2018). [DOI]
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❖ **Materialism Podcast Episodes** (co-authors Taylor D. Sparks and Andrew Falkowski)

1. "PHAs and Biodegradable Plastic," *Materialism Podcast*, April 2024.
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❖ Non-Research Publications:

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