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

Submitted

1. Stanley Loa, Sterling G. Baird*, Joshua Schrier, Ben Blaiszik, Sergei V. Kalinin, Helen, Tran, **Taylor D. Sparks**, Alán Aspuru-Guzik "Review of Low-cost Self-driving Laboratories: The "Frugal Twin" Concept" *under review*.
2. Christopher M. Collins[†], Hasan M. Sayeed*[‡], 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*.
3. 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*.
4. Hasan M. Sayeed* and **Taylor D. Sparks** "Structural feature vectors derived from word embeddings of RoboCrystallographer descriptions" *under review*.
5. 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*.
6. 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*.
7. Pooya Elahi*, Anil V. Virkar, **Taylor D. Sparks**, and Michael Simpson "Electrolyte degradation in Yttria Stabilized Zirconia Solid Oxide Electrolyzer Cells" *under review*.

Accepted or published

1. 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" *accepted to Digital Discovery on December 28 2023*.
2. 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" *accepted to Matter December 18 2023*.
3. 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" *published online Digital Discovery on Dec 6th 2023.* [DOI]
4. 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]
5. **Taylor D. Sparks** "Tales from Sabbatical III: Coming Home" *Matter*, **6** [12], 4111-4115 (2023). [DOI]
6. 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]
7. 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]
8. 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]

9. 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]
10. 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]
11. Kaitlin Tyler, Enze Chen, Bryce Meredig, and **Taylor D. Sparks** "Artificial intelligence in materials education: A roundtable discussion" *JOM*, **75**, 2083-2085 (2023). [DOI]
12. 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]
13. 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]
14. 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]
15. Sterling G. Baird*, Jason R. Hall*, and **Taylor D. Sparks** "Compactness Matters: Improving Bayesian Optimization Efficiency of Materials Formulations through Invariant Search Spaces" *Computational Materials Science*, **224**, 112134 (2023). [DOI]
16. 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]
17. 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]
18. **Taylor D. Sparks** "Tales from Sabbatical II: During your stay" *Matter*, **6** [3], 648-652 (2023). [DOI]
19. 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]
20. 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]
21. 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]
22. 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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25. 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]
26. 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]
27. 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]

28. (invited) **Taylor D. Sparks** "Tales from Sabbatical I: Planning your leave" *Matter,* **5** [6], 1623-1626 (2022). [DOI]
29. 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]
30. 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]
31. 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]
32. 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]
33. (invited) Sterling G. Baird*, Marianne Liu*, Hasan M. Sayeed*, and **Taylor D. Sparks** "Data-Driven Materials Discovery and Synthesis using Machine Learning Methods" *Comprehensive Inorganic Chemistry III, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering,* (2022) [DOI].
34. (invited) Sterling G. Baird*, Tran Diep*, and **Taylor D. Sparks** "DiSCoVeR: a Materials Discovery Screening Tool for High Performance, Unique Chemical Compositions" *Digital Discovery*, **1**, 226-240 (2022). [DOI]
35. **Taylor D. Sparks** "Inaugural Congress to Focus on Artificial Intelligence" *JOM*, **73**, 3679-3680 (2021). [DOI]
36. 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]
37. Debanshu Banerjee* and **Taylor D. Sparks** "Comparing transfer learning to feature optimization in microstructure classification" *iScience,* **25**, [2], 103774 (2021). [DOI]
38. 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]
39. 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]
40. 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]
41. Anthony Yu-Tang Wang*, Steven K. Kauwe*, Ryan Murdock*, and **Taylor D. Sparks** "Compositionally-Restricted Attention-Based Network for Materials Property Prediction," *npj Computational Materials,* **7**, 77 (2021). [DOI]
42. **Taylor D. Sparks** and Debanshu Banerjee* "Materials Informatics and Polymer Science: Pushing the Frontiers of our Understanding" *Matter*, **4** [5], 1454-1456 (2021). [DOI]
43. 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]

44. **Taylor D. Sparks**, Anton Oliynyk, and Vitaliy Romaka "Preface to the special issue on machine learning and data-driven design of materials issue in computational materials science" *Computational Materials Science,* **195**, 110452 (2021). [DOI]
45. (invited) Marianne Liu*, Conrad Clement*, Kathy Liu, Xuming Wang, and **Taylor D. Sparks** "A Data Science Approach for Advanced Solid Polymer Electrolyte Design," *Computational Materials Science,* **187**, 110108 (2020). [DOI]
46. 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]
47. (invited) Amber Barron* and **Taylor D. Sparks** "Commercial Marine-degradable Polymers for Flexible Packaging" *iScience,* **23**, 101353, (2020). [DOI]
48. 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]
49. (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]
50. Jason Nance* and **Taylor D. Sparks** "From Streetlights to Phosphors: a Review on the Visibility of Roadway Markings," *Progress in Organic Coatings,* **148**, 105749 (2020). [DOI]
51. Conrad Clement*, Steven K. Kauwe*, and **Taylor D. Sparks** "Benchmark AFLOW Data Sets for Machine Learning," *Integrating Materials and Manufacturing Innovation,* 9, 153-156 (2020). [DOI]
52. Jason Nance* and **Taylor D. Sparks** "Comparison of Coatings for $SrAl_2O_4$:Eu^{2+},Dy^{3+} powder in Waterborne Road Striping Paint under Wet Conditions" *Progress in Organic Coatings,* **148**, 105749 (2020). [DOI]
53. Brennan Theler*, Steven K. Kauwe*, and **Taylor D. Sparks** "Materials abundance, price, and availability data from the years 1998 to 2015" *Integrating Materials and Manufacturing Innovation*, **9**, 144-150 (2020). [DOI]
54. (invited) Andrew R. Falkowski* and **Taylor D. Sparks** "The Materialism podcast: Exploring new avenues for materials science education" *Matter*, **2**, [2] 276-278 (2020). [DOI]
55. (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]
56. Su Kong Chong, Ryuichi Tsuchikawa, Jared Harmer, **Taylor D. Sparks**, and Vikram V. Deshpande "Landau Levels of Topologically-Protected Surface States Probed by Dual-Gated Quantum Capacitance" *ACS Nano* **14**, [1], 1158-1165 (2020). [DOI]
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Reference Electrodes in Proton Exchange Membrane Fuel Cells" *Journal of the Electrochemical Society*, **166**, [12], F784-F795 (2019). [DOI]

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66. Benjamin Gilmore*, Zachary Luscher*, Kyle Roberts, George Fisher, and **Taylor D. Sparks** "Comparison of fatigue in fiber-backed PVDF and PFA fluoropolymer linings" *Polymer Degradation and Stability,* **162**, 122-128 (2019). [DOI]
67. (invited) Steven K. Kauwe*, Trevor David Rhone, and **Taylor D. Sparks** "Data-driven studies of lithium-ion-battery materials" *Crystals*, **9**, [1] 54 (2019). [DOI]
68. Shadi Al Khateeb* and **Taylor D. Sparks** "Spray pyrolysis of conductor and binder free porous FeS2 films for high performance lithium ion batteries" *Journal of Materials Science,* **54**, [5], 4089-4104 (2019). [DOI]
69. Isaac Nelson, Taylor A. Ogden, Shadi Al Khateeb*, Jake Graser*, **Taylor D. Sparks**, Jake J. Abbott, and Steven E. Naleway "Freeze casting of surface-magnetized Fe3O4 particles with a Helmholtz coil in a unidirectional static magnetic field to fabricate materials inspired by bone" *Advanced Engineering Materials*, 1801092, (2018). [DOI]
70. Kyu-Bum Han*, Su Kong Chong, Anton O. Oliynyk, Akira Nagaoka, Suzanne Petryk*, Michael Scarpulla, Vikram Deshpande, and **Taylor D. Sparks** "Enhancement in surface mobility and quantum transport of Bi2−xSbxTe3−ySey topological insulator by controlling the crystal growth conditions" *Scientific Reports*, 8:17290 (2018). [DOI]
71. Su Kong Chong, Kyu Bum Han*, Akira Nagaoka, Ryuichi Tsuchikawa, Renlong Liu, Haoliang Liu, Z. Valy Vardeny, Dmytro A. Pesin, Changgu Lee, **Taylor D. Sparks** and Vikram V. Deshpande "Topological Insulator-Based van der Waals Heterostructures for Effective Control of Massless and Massive Dirac Fermions" *Nano Letters*, **18**, [12], 8047-8053 (2018). [DOI]
72. Dong Zhang, Anton O. Oliynyk, Gabriel M. Duarte, Abishek K. Iyer, Leila Ghadbeigi*, Steven K. Kauwe*, **Taylor D. Sparks**, and Arthur Mar "Not Just Par for the Course: Over 72 Quaternary Germanides RE4M2XGe4 (RE = La–Nd, Sm, Gd–Tm, Lu; M = Mn–Ni; X = Ag, Cd) and the Search for Intermetallics with Low Thermal Conductivity" *Inorganic Chemistry*, **57**, [22], 14249-14259 (2018). [DOI]
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75. Jake Graser*, Steven K. Kauwe*, and **Taylor D. Sparks** "Machine learning and energy minimization approaches for crystal structure predictions: A review and new horizons" *Chemistry of Materials,* **30**, [11], 3601-3612, (2018). [DOI].
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77. Kyu-Bum Han*, Jake Graser*, Alexandre Stella*, John Fuertez, Van Nguyen, John McLennan, and **Taylor D. Sparks** "Calcium alginate polymer encapsulation of proppant with time-release delivery of microbial consortia for methanogenesis" *Hydraulic Fracturing Journal,* **5**, [3], 62-74 (2018).

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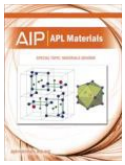

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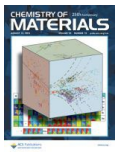

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❖ **Conference Proceedings: (underlined names are undergraduate co-authors)**

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2. Logan G. Kiefer, Andrew R. Falkowski, and **Taylor D. Sparks** "Electroplating of thin films" JoVE Science Education Database. Inactive Collection. JoVE, Cambridge, MA, (2018). [DOI]
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. "Radar Absorbing Materials," *Materialism Podcast*, February 2024.
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15. "Thermal Spray Coatings at General Electric," *Materialism Podcast*, June 2023.
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❖ Non-Research Publications:

1. **Taylor D. Sparks** "Materials Informatics: Reducing Trial & Error from the Discovery of New Materials" TEDxSaltLakeCity, September 22 2019, published online at TED.com
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