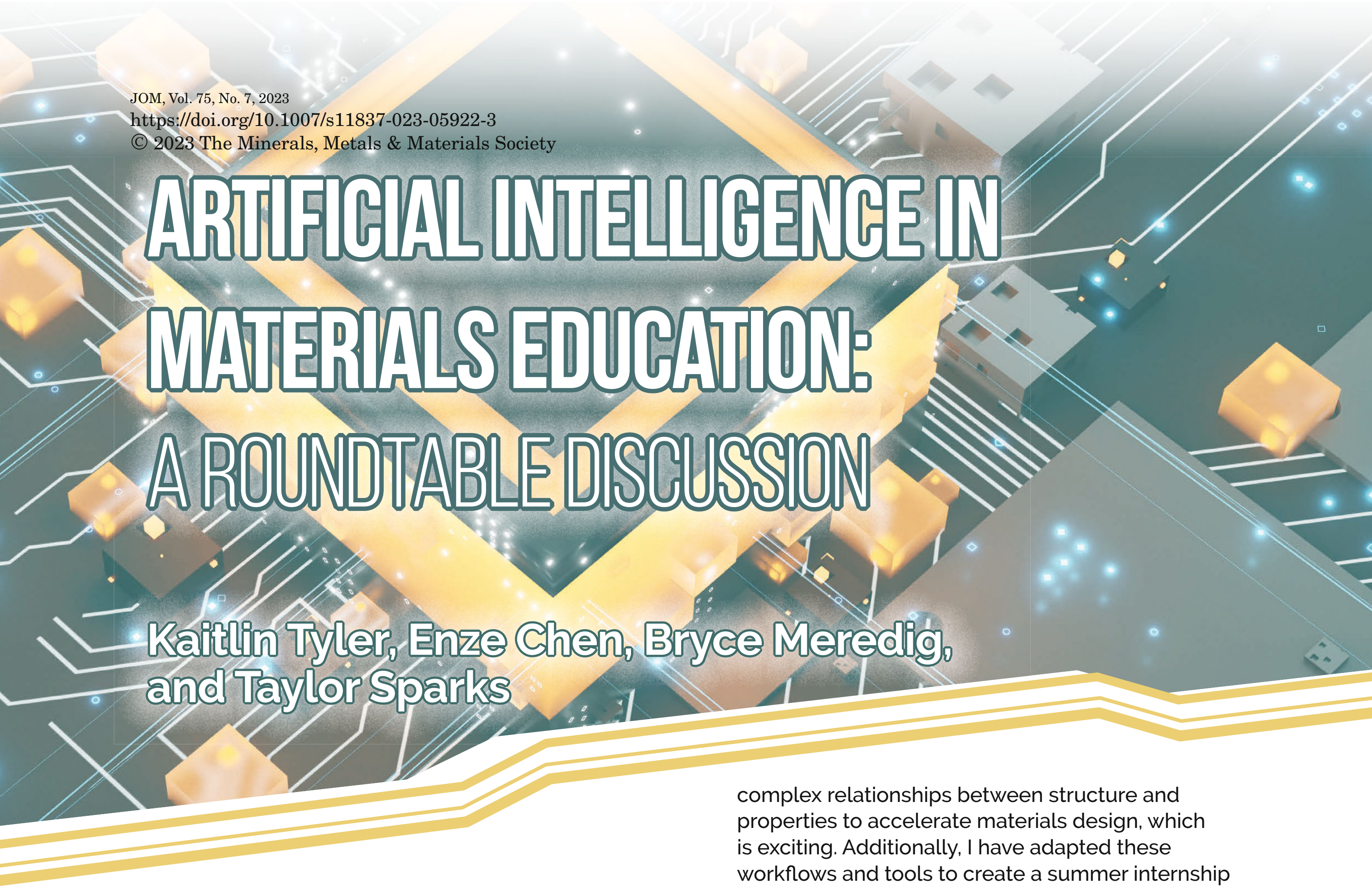

JOM, Vol. 75, No. 7, 2023
https://doi.org/10.1007/s11837-023-05922-3

ARTIFICIAL INTELLIGENCE IN MATERIALS EDUCATION: A ROUNDTABLE DISCUSSION

Kaitlin Tyler, Enze Chen, Bryce Meredig, and Taylor Sparks

Editor's Note: In this roundtable conversation, *Kaitlin Tyler*, *JOM* liaison for the TMS Education Committee, poses questions about the role that artificial intelligence (AI) and machine learning can play in materials and how these tools can be incorporated into the classroom. Respondents are *Enze Chen*, a Ph.D. candidate at the University of California, Berkeley; *Bryce Meredig*, independent consultant; and *Taylor Sparks*, associate professor of materials science and engineering at the University of Utah.

Kaitlin Tyler: How do you currently use AI and machine learning in your job?

Bryce Meredig: I help science and engineering organizations use AI, and computation more broadly, to reach their goals more efficiently.

Taylor Sparks: My research group is founded on the use of AI and machine learning as tools to aid in materials discovery. We use these tools to help us narrow the search space for new alloys, compounds, and formulations.

Enze Chen: For my thesis, I use atomistic simulations and machine learning to study planar defects in structural alloys, where I have built machine learning models to predict the antiphase boundary energy in nickel-based superalloys and other interfacial properties in α-titanium alloys. Here, the overarching goal is to use machine learning to capture the complex relationships between structure and properties to accelerate materials design, which is exciting. Additionally, I have adapted these workflows and tools to create a summer internship curriculum for undergraduates from traditionally underrepresented backgrounds in engineering. It has been a joy to work with them in data-driven design of high-κ dielectrics as they learn about how advanced machine learning tools are used to drive materials R&D.

Tyler: In a few words, how would you describe AI and how it relates to materials?

Chen: AI is a clever tool for solving materials challenges.

Meredig: AI is a powerful tool that helps us focus our limited resources where they are most likely to pay off. In materials development, for example, we can use AI to identify the most promising candidates and avoid investing in dead ends.

Sparks: Material science as a discipline is built on this idea of capturing and exploiting relationships between materials processing, properties, and structure. AI allows us to find and exploit much more subtle nuanced relationships or higher order ones where humans really struggle.

Tyler: What value do you see AI providing the materials community?

Sparks: Artificial intelligence and machine learning can drastically reduce the number of experiments necessary before we find materials with desired properties. We can reduce the cost and time to innovation and even deployment. These tools can also help us construct valuable surrogate models for predicting properties that were otherwise really difficult for us to build empirical models for.

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Chen: Fundamentally, I see AI as another tool—albeit a novel and powerful one—to add to our toolbox for designing new materials. I've seen its value in automating tasks and identifying multidimensional relationships across materials domains, and this mostly stems from the fresh perspectives AI provides from disparate fields of engineering. In a world where knowledge feels increasingly siloed, it's uplifting to see the productive synergy between AI and materials. We should be tactful about its use as it often produces specious results, but I believe advancements in AI will ultimately enable us to excel at what we do best: identifying processing, structure, properties, and performance relationships across scales to design new materials to benefit society.

Tyler: When you talk about AI with other materials scientists and materials educators, what reaction do you get most often?

Meredig: A mixture of excitement and some skepticism. People are always eager to have a new tool that makes their job easier, but they also are cautious of the hype surrounding AI. That's why it's important to be realistic when describing what AI is and is not good for in materials science.

Chen: I would say skepticism, which makes sense. Five years ago, there was skepticism and fear about AI taking over our jobs due to uncertainties around the new technology. Now, people are no less skeptical, but it's about building trust in the results of AI. I'm a big fan of healthy skepticism that kindles further conversation and progress, but it seems that many people who want to learn more about AI are unsure where to start. This is why I am committed to working at the intersection of AI, materials, and education, and to developing domain-specific educational resources to help move the field forward.

Sparks: The reaction from other material scientists has really changed over time. Ten years ago, when I was starting as a new faculty member and proposing the use of materials and informatics as a tool, there was much more skepticism. There were some that did not even consider it as a part of material science. That has really changed. There have been some high-profile success stories, and people are becoming more familiar with the limitations but also the capabilities of machine learning tools as well. Nowadays, people see it as a useful tool, but there is less surprise about what it is capable of doing.

Tyler: What skills related to AI/machine learning does the next generation of engineers need to know?

Chen: I think about this question a lot, and it's hard to answer because AI and machine learning change so quickly. I believe all engineers could benefit from standard proficiency in AI discourse placed in the context of materials. Regardless of one's role, they'll likely interface with people who work with AI/machine learning, and this fluency will facilitate the collaboration/interactions. More importantly, I view the current AI race as a fervid chase for better answers, and it's unclear to me if we're spending enough time asking better questions. As great as the resulting AI tools may be, they're useless if we're answering the wrong questions. I would like to help the next generation of engineers develop the ability to ask meaningful questions to guide the strategic use of AI solutions in materials.

Sparks: For material scientists to really leverage the power of machine learning and materials informatics, it is critical that they improve their coding ability and their fundamental knowledge of statistics. There is no substitute for learning the fundamentals of linear algebra and probability if you're going to be developing new tools. If you're going to be using existing tools, I think that the barrier to entry is dropping every day. It's getting fairly routine.

Meredig: The next generation of materials scientists should definitely learn how to use AI in their day-to-day activities. The nature of every role in our field, not just computational work, will be transformed at least to some extent by AI. Related skills in coding, statistics, and data science will continue to grow in importance in materials science.

INDUSTRY IS DEMANDING THIS SKILL SET FROM OUR STUDENTS. WE NEED TO BE TRAINING THEM SO THAT THEY ARE RESPONSIVE TO THE NEEDS OF FUTURE CAREERS.

Tyler: To those who are nervous about including AI in their classroom, do you have any words of encouragement?

Sparks: Whether we are nervous or not is sort of irrelevant at this point. Industry is demanding this skill set from our students. We need to be training them so that they are responsive to the needs of future careers. For those that are worried that they don't have the right skill set themselves to teach it, I would point out that there have never been more awesome resources for learning these tools. There are great best practices articles, example notebooks, powerful libraries and open source packages, hackathons and workshops, and even YouTube tutorials.

Meredig: I encourage educators to embrace this opportunity and help students channel their excitement for AI toward challenges in materials science. Society is counting on our field for solutions to urgent problems, such as climate change, and AI can help us deliver those solutions faster.

Chen: AI is cool, and so are you! As educators, one of the best ways to serve our students is to help them navigate the volatile world of AI by focusing on the course learning goals and what students need to be successful. Sometimes AI is the answer, but in many cases it's not, and your course will be better off without it. If I choose to include AI, I know that it will not replace the students' creativity, but rather give them more freedom to exercise it. And if AI has already found its way in, don't let it replace you; rather, let it work for you. Use AI-written assignments as teachable moments or exercises in fact-checking to continue cultivating a classroom culture of trust and authenticity.

MEET THE PANELISTS

Enze Chen

Enze Chen is a Ph.D. candidate in Materials Science and Engineering (MSE) at the University of California, Berkeley. As a National Science Foundation Fellow, he works at the intersection of materials, computing, and education, where he pursues parallel research tracks studying planar defects in structural alloys and the integration of computational tools in MSE education. He is passionate about teaching and mentoring and is a recipient of the UC Berkeley Outstanding Graduate Student Instructor Award and MSE Graduate Student Equity and Inclusion Award.

Taylor Sparks

Taylor Sparks is an associate professor of materials science and engineering at the University of Utah and currently a Royal Society Wolfson Visiting Fellow on sabbatical at the University of Liverpool. He holds a B.S. in materials science and engineering from the University of Utah, M.S. in materials from the University of California Santa Barbara, and Ph.D. in applied physics from Harvard University. He was a recipient of the National Science Foundation CAREER Award and a speaker for TEDxSaltLakeCity.

Bryce Meredig

Bryce Meredig is a consultant, researcher, and entrepreneur in the field of materials AI and computation. He co-founded Citrine Informatics in 2013, serving as chief executive officer and later chief science officer, helping to grow the company over nearly a decade into a leading provider of enterprise materials informatics software. Meredig earned his BAS and MBA at Stanford University, and his Ph.D. in materials science and engineering at Northwestern University.

Kaitlin Tyler

Kaitlin Tyler is currently an academic content development program manager at Ansys, with an emphasis on materials-related topics. Her role focuses on supporting academics using Ansys software in the classroom through engaging educational resources. She received her Ph.D. at the University of Illinois Urbana-Champaign in 2018. She is currently the *JOM* liaison for the TMS Education Committee and a member of the TMS Diversity, Equity, and Inclusion Committee.