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TOPICAL REVIEW

Generative artificial intelligence for discovering new materials

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https://doi.org/10.61109/cs.202410.134

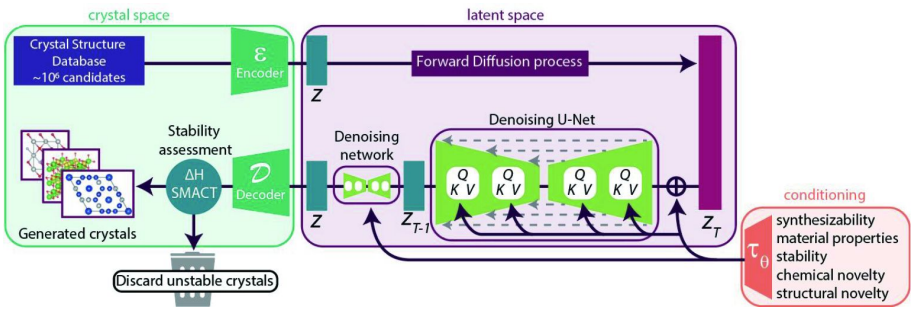
Citation: T.D. Sparks, Generative artificial intelligence for discovering new materials, *Coshare Science* **02**, 07 (2024)

Author introduction

Dr. Sparks is a professor of Materials Science and Engineering at the University of Utah and recently completed a sabbatical at the University of Liverpool with support from the Royal Society Wolfson Visiting Fellow program. He holds a BS in MSE from the UofU, MS in Materials from UCSB, and PhD in Applied Physics from Harvard University. He was a recipient of the NSF CAREER Award and a speaker for TEDxSaltLakeCity. He is active in MRS, TMS, and ACERS societies and has served as an Associate Editor for the journals *Computational Materials Science* and *Data in Brief*. He is the Editor-in-Chief elect for the *Integrating Materials and Manufacturing Innovation*. When he's not in the lab you can find him running his podcast "Materialism," creating materials educational content for his YouTube channel, or canyoneering with his 4 kids in southern Utah.

Highlights

- High-throughput screening is not the same as materials discovery.
- Generative machine learning is unlocking true discovery.
- Many models exist, but these share some common approaches and limitations.
- New approaches will leverage crystal graphs, reinforcement learning, and language models.



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·Materials science·
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Abstract Crystal structure prediction has long fascinated scientists. There has been intense investigation over the last century ranging from simplistic rules to data-driven predictions and, most recently, generative artificial intelligence tools developed by academics and now deployed at scale by private companies like DeepMind. The author describes the timeline of crystal structure prediction and how machine learning has supplemented and, in some cases, replaced traditional approaches. The video article compares generative models including variational autoencoders, generative adversarial networks, and diffusion models and describes new efforts to condition these models to achieve inverse design of new crystal structures. Specific examples of xtal2png and CrysTens representations were given.

Keywords generative machine learning, materials discovery, inverse design, modeling, high throughput, materials informatics

Acknowledgements This work was supported by the National Science Foundation under grant no. DMR-1651668 and DMR-1950589. The work was also supported by the Army Research Office Materials Design program under contract number #W911NF-23-1-0333.

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Submitted: 8 October 2024; Accepted: 28 October 2024; Published Online: 31 October 2024