Advancing reticular chemistry with large language models

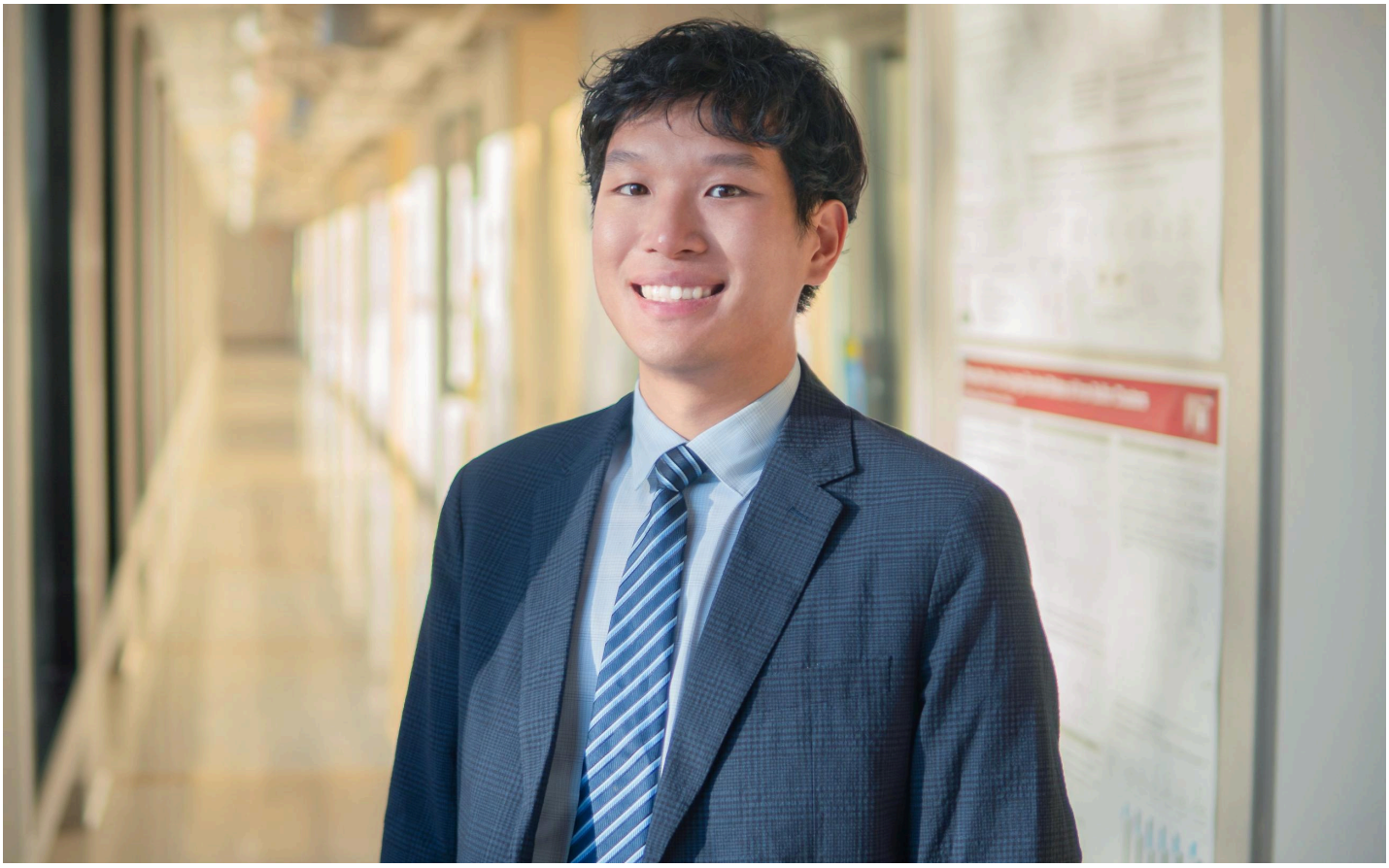
by Tiffany Lohwater | Berkeley Computing, Data Science, and Society *February 27, 2025*

UC Berkeley researchers in chemistry and computer science recently reported on their use of an AI tool – large language models – to advance discovery in reticular chemistry and materials science.

The perspective paper (https://www.nature.com/articles/s41578-025-00772-8) was published in the journal *Nature Reviews Materials* earlier this month by researchers at the Bakar Institute of Digital Materials for the Planet (BIDMaP) and the Department of Chemistry at Berkeley. BIDMaP is part of Berkeley's College of Computing, Data Science, and Society.

By leveraging generative AI to help streamline routine laboratory tasks, the researchers said, chemists can be further empowered to address societal issues such as climate change and clean air and water.

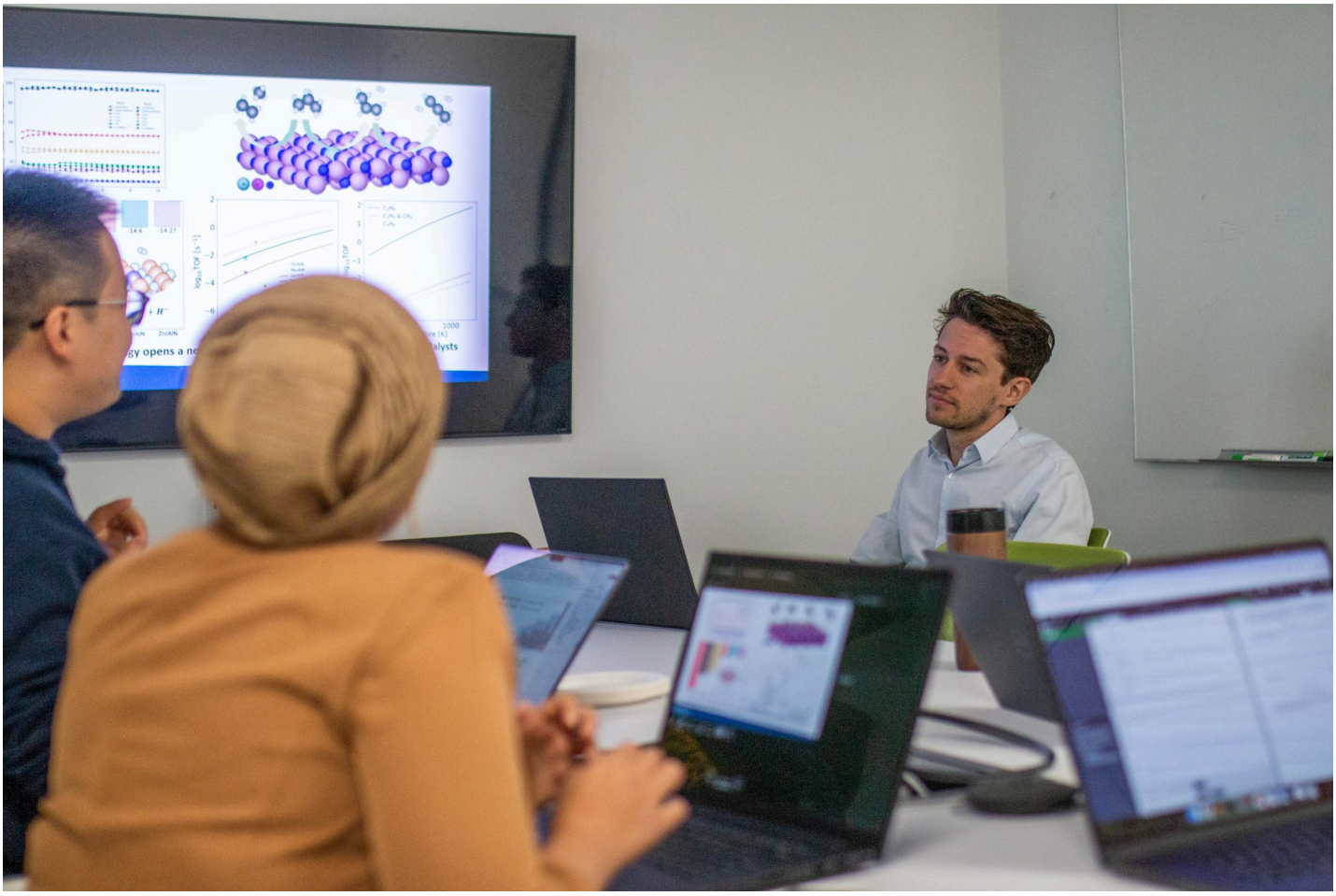
"Reticular chemistry involves the design and synthesis of intricate, extended structures and is highly data-driven," said Zach Zheng (https://bidmap.berkeley.edu/people/zhiling-zach-zheng), a BIDMaP postdoctoral fellow who recently wrote about his personal journey (https://pubs.acs.org/doi/10.1021/acscentsci.4c01838?articleRef=test) in science. "Large language models (LLMs) can serve as computational decision-makers, enhancing automated synthesis by interfacing with various experimental platforms – planning reactions, transferring solutions and characterizing results."



Zach Zheng is a postdoctoral fellow at the Bakar Institute of Digital Materials for the Planet. (Photo / Zach Zheng)

Zheng collaborated with postdoctoral fellows and co-authors Nakul Rampal (https://bidmap.berkeley.edu/people/nakul-rampal) and Théo Jaffrelot Inizan (https://bidmap.berkeley.edu/people/theo-jaffrelot-inizan) on the research. BIDMaP faculty Omar Yaghi (https://vcresearch.berkeley.edu/faculty/omar-yaghi), Christian Borgs (https://bidmap.berkeley.edu/people/christian-borgs) and Jennifer Chayes (https://cdss.berkeley.edu/people/jennifer-chayes) were also co-authors on this paper.

The paper explains how “chemistry-aware” LLMs can be directed and fine-tuned to undertake specific tasks – such as data mining from the scientific literature – and integrated into existing practices of reticular chemistry.



Postdoctoral fellow Théo Jaffrelot Inizan (right) meets with BIDMaP researchers. (Photo / Kayla Sim / UC Berkeley College of Computing, Data Science, and Society)

Zheng, Rampal and Inizan noted the team's findings should be vastly transferable to other material science fields and encouraged researchers to explore the use of AI tools to further scientific discovery.

"LLMs developed with domain knowledge can rapidly analyze hundreds of papers, extract synthesis parameters, and predict material properties, making them invaluable research assistants," said Zheng.

Source: Berkeley Computing, Data Science, and Society
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