Machine learning accelerates discovery of materials for use in industrial processes

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Artificial intelligence enabled autonomous design of nanoporous materials.

Credit: University of Toronto

New research led by researchers at the University of Toronto (U of T) and Northwestern University employs machine learning to craft the best building blocks in the assembly of framework materials for use in a targeted application.

The findings, published today in *Nature Machine Intelligence*, demonstrated that the use of artificial intelligence (AI) approaches can help in proposing novel materials for diverse applications. One example is the separation of carbon dioxide from industrial combustion processes. AI approaches promise the acceleration of the design cycle for materials.

With the objective of improving the separation of chemicals in industrial processes, the team of researchers—including collaborators from Harvard University and the University of Ottawa—set out to identify the best reticular frameworks (e.g., metal organic frameworks, covalent organic frameworks) for use in the process. Such frameworks, which can be thought of as tailored molecular "sponges", form via the self-assembly of molecular building blocks into different arrangements and represent a new family of crystalline porous materials that have been proven to be promising in addressing many technology challenges (e.g., clean energy, sensoring, biomedicine, etc.)

"We built an automated materials discovery platform that generates the design of various molecular frameworks, significantly reducing the time required to identify the optimal materials for use in this particular process," says Zhenpeng Yao, a postdoctoral fellow in the Departments of Chemistry and Computer Science in the Faculty of Arts & Science at U of T, and lead author of the study. "In this demonstrated employment

of the platform, we discovered frameworks that are strongly competitive against some of the best-performing materials used for CO_2 separation known to date."

The perennial challenges in addressing CO_2 separation and other problems like greenhouse gas reduction and vaccine development, however, are the unpredictable amount of time and extensive trial-and-error efforts required in the pursuit of such new materials. The occasionally infinite combinations of molecular building blocks available in the construction of chemical compounds can mean the exhaustion of significant amounts of time and resources before a breakthrough is made.

"Designing reticular materials is particularly challenging, as they bring the hard aspects of modeling crystals together with those of modeling molecules in a single problem," says senior coauthor Alán Aspuru-Guzik, Canada 150 Research Chair in Theoretical Chemistry in the Departments of Chemistry and Computer Science at U of T and Canada CIFAR AI Chair at the Vector Institute. "This approach to reticular chemistry exemplifies our emerging focus at U of T of accelerating materials development by means of artificial intelligence. By using an AI model that can 'dream' or suggest novel materials, we can go beyond the traditional library-based screening approach."

The researchers focused on the development of metal-organic frameworks (MOFs) that are now considered the ideal absorbing material for the removal of CO_2 from flue gas and other combustion processes.

"We began with the construction of a large number of MOF structures on the computer, simulated their performance using molecular-level modeling, and built a training pool applicable to the chosen application of CO_2 separation," said study co-author Randall Snurr, the John G.

Searle Professor and chair of the Department of Chemical & Biological Engineering in the McCormick School of Engineering at Northwestern University. "In the past, we would have screened through the pool of candidates computationally and reported the top candidates. What's new here is that the automated materials discovery platform developed in this collaborative effort is more efficient than such a "brute force" screening of every material in a database. Perhaps more importantly, the approach uses machine learning algorithms to learn from the data as it explores the space of materials and actually suggests new materials that were not originally imagined."

The researchers say the model shows great prediction and optimization capability in the design of novel reticular frameworks, particularly in combination with already known candidates in specific functions, and that the platform is fully customizable in its application to address many contemporary technology challenges.

More information: Zhenpeng Yao et al, Inverse design of nanoporous crystalline reticular materials with deep generative models, *Nature Machine Intelligence* (2021). DOI: 10.1038/s42256-020-00271-1

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