AI lights the way for futuristic electronics, from bendy TVs to lightweight solar cells

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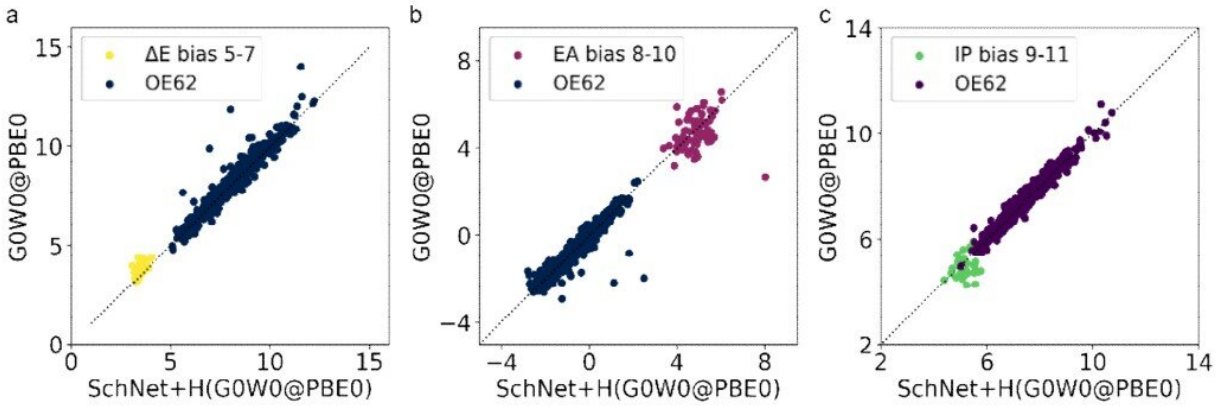

Validation of electronic properties of generated molecules. a) Fundamental gaps, ΔE, b) electron affinities, EA, and c) ionization potentials, IP, for molecules of the original data set and G-SchNet generated structures of the last 3 biasing steps predicted with SchNet+H and computed with G0W0@PBE0. Credit: *Nature Computational Science* (2023). DOI: 10.1038/s43588-022-00391-1

Artificial intelligence (AI) is transforming modern electronics—accelerating the design of bendable TV screens, ultra-lightweight revolutionized solar cells and more.

In a study published in *Nature* February 6, scientists used a type of AI algorithm to create new molecules, suited for electronics that could come straight from a sci-fi movie. The algorithm is able to rapidly

design millions of previously undiscovered molecules by building them atom by atom on a computer.

Generative deep learning methods have become popular to create "deep fakes" of images and even computer-generated music. The application of generative AI in the context of chemistry is very recent and has the potential to reshape scientific discovery. Finding molecules with optimal properties in the lab, through human trial and error, would otherwise be like finding a needle in a haystack.

The use of AI enables a form of molecular design driven by the material's intended use. Generative deep learning is able to create three-dimensional molecules that satisfy certain criteria much more efficiently than any previous technique. In this study, led by the University of Warwick, the authors train the AI to search for molecules that can absorb and emit light of a certain color and are also easy to synthesize in the lab. The corresponding molecules can also be designed to be small and suitable for mass production, promising to make newer generations of flexible TVs and screens cheaper, more flexible, lightweight and with higher color brilliance.

Reinhard Maurer, Professor of Computational Surface Chemistry and Interface Physics, at the University of Warwick, who led the study, said, "Our study developed an algorithm that can focus on a narrow range of electronic and optical properties, proposing new molecules for electronics applications. Initially, the algorithm would only generate nonsensical molecules, until we trained it to ensure that the molecules can be easily made in the lab. The approach can help to optimize electronic and optical properties of organic molecules that can be used in organic light emitting diodes (OLEDS) which go into flexible displays and molecules for solar cells."

According to Professor Maurer, AI to support design and discovery is

starting to play an important role in science: "Modern materials are too complex for lab-based trial and error search. AI-driven computational design can help to propose brand new molecules but also optimize existing ones. Possible application areas for property-driven design go well beyond electronics. The process could help to design new drugs by predicting the solubility of molecules or their ability to bind to enzymes, both important properties of pharmaceuticals."

More information: Julia Westermayr et al, High-throughput property-driven generative design of functional organic molecules, *Nature Computational Science* (2023). DOI: 10.1038/s43588-022-00391-1

Provided by University of Warwick