Artificial intelligence ARTIST instantly captures materials' properties

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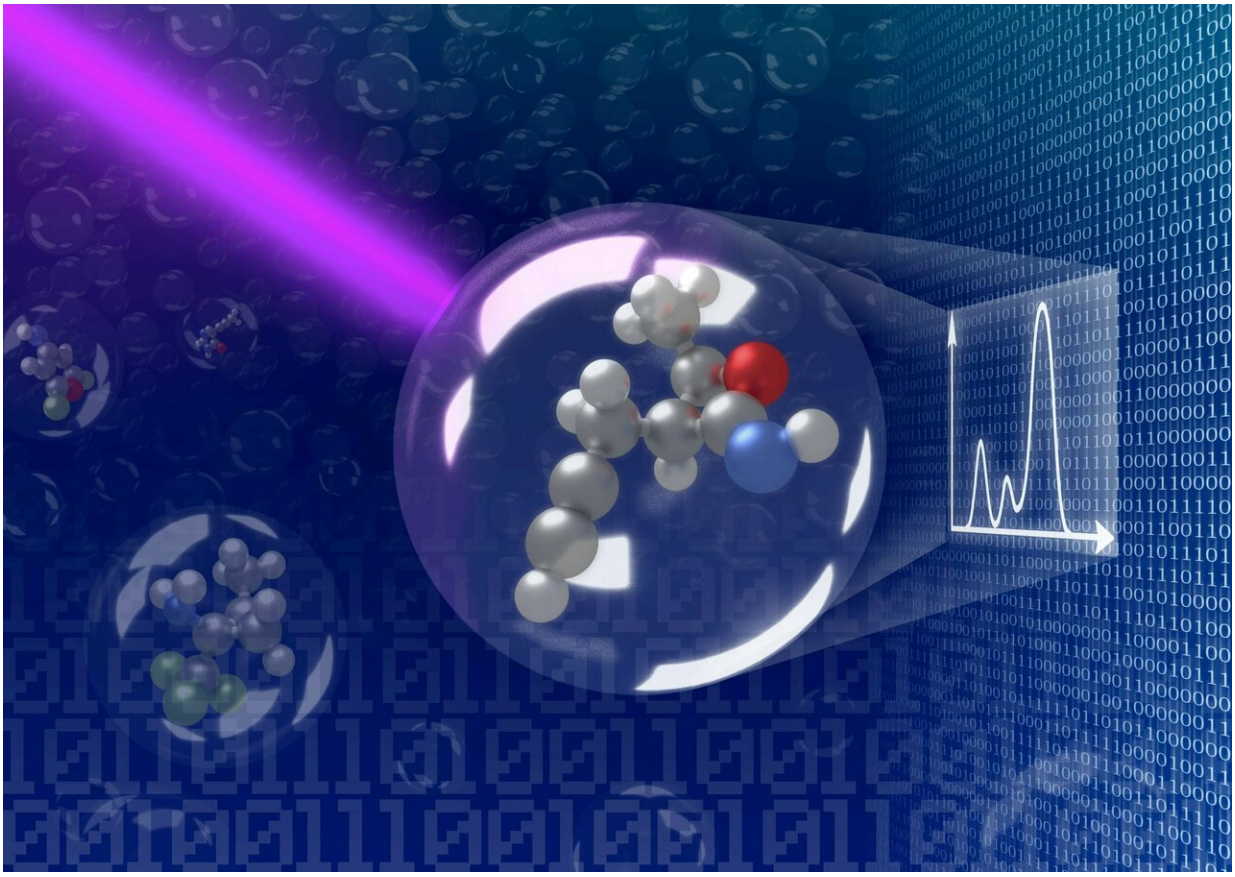

ARTIST, which stands for Artificial Intelligence for Spectroscopy, instantly determines how a molecule will react to light. Credit: Jari Järvi/Aalto University

Researchers at Aalto University and the Technical University of

Denmark have developed an artificial intelligence (AI) to seriously accelerate the development of new technologies from wearable electronics to flexible solar panels. ARTIST, which stands for Artificial Intelligence for Spectroscopy, instantly determines how a molecule will react to light—clinch-pin knowledge for creating the designer materials needed for tomorrow's technology.

Scientists traditionally study molecular reactions to external stimuli with spectroscopy, a widely used method across the natural sciences and industry. Spectroscopy probes the internal properties of materials by observing their response to, for example, light, and has led to the development of countless everyday technologies. Existing experimental and computational spectroscopy approaches can be, however, incredibly costly. Time in highly specialised laboratories is expensive and often severely limited, while computations can be tedious and time-intensive.

With ARTIST, the research team offers a paradigm shift to how we determine the spectra—or response to light—of individual molecules.

"Normally, to find the best molecules for devices, we have to combine previous knowledge with some degree of chemical intuition. Checking their individual spectra is then a trial-and-error process that can stretch weeks or months, depending on the number of molecules that might fit the job. Our AI gives you these properties instantly," says Milica Todorovic, a postdoctoral researcher at Aalto University.

With its speed and accuracy, ARTIST has the potential to speed up the development of flexible electronics, including light-emitting diodes (LEDs) or paper with screen-like abilities. Complementing basic research and characterization in the lab, ARTIST may also hold the key to producing better batteries and catalysts, as well as creating new compounds with carefully selected colours.

The multidisciplinary team trained the AI in just a few weeks with a dataset of more than 132,000 organic molecules. ARTIST can predict with exceedingly good accuracy just how those molecules—and those similar in nature—will react to a stream of light. The team now hopes to expand its abilities by training ARTIST with even more data to make an even more powerful tool.

"Enormous amounts of spectroscopy information sit in labs around the world. We want to keep training ARTIST with further large datasets so that it can one day learn continuously as more and more data comes in," explains Aalto University Professor Patrick Rinke.

The researchers aim to release ARTIST on an open science platform in 2019, and it is currently available for use and further training upon request.

More information: Kunal Ghosh et al. Deep Learning Spectroscopy: Neural Networks for Molecular Excitation Spectra, *Advanced Science* (2019). DOI: 10.1002/advs.201801367

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