AI developed by a group of researchers at Aalto University could significantly speed up the search for new materials.

Espoo, Finland - October 5, 2017: New materials which are designed specifically for a particular task, such as materials for mobile phone batteries which can hold charge for a long time, are everywhere around us. A group of researchers from the machine learning and applied physics departments at Aalto University, School of Science, have used an artificial intelligence (AI) algorithm to predict molecular properties. The AI, powered by deep neural networks, makes the prediction using as input only the shape and atomic composition of molecules. The neural networks can predict these properties, for individual molecules, in milliseconds compared to minutes taken by traditional techniques. The algorithm has also achieved state-of-the-art results in predicting the molecular orbital[1] energies and is the first[2] to predict molecular spectra.

When searching for new materials, scientists usually start with a large database of potential molecules. A crucial first step is to study each molecule individually looking for properties favourable for the intended application of the final material. The molecular spectra help scientists identify these properties and conventionally, computer simulations have been used to compute them. Since the simulations are repeated for each molecule the traditional methods are slow. The AI, on the contrary, learns the spectra from a large database of pre-computed molecule-spectra pairs. The database of molecule-spectra pairs is quite time consuming to generate since they are computed using traditional techniques. Also the AI can take a few days to learn from the data. However, once the learning is complete the AI can predict spectra for new molecules in milliseconds. Given that the AI needs to learn from data only once (or very sparingly) it is therefore much faster[3] overall.

The researchers compared their proposed algorithm to the previous state-of-the-art and found their method to give higher prediction accuracy while predicting molecular orbital energies. The molecular orbital energies are closely related to the spectra discussed above and accuracy in predicting them has been used as a benchmark by other researchers working in this domain.

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[1] Specifically, the sixteen highest occupied molecular energies (HOMO)
[2] First AI to make spectra predictions.
[3] Compared to traditional techniqes.