Bonding's next top model: Projecting bond properties with machine learning

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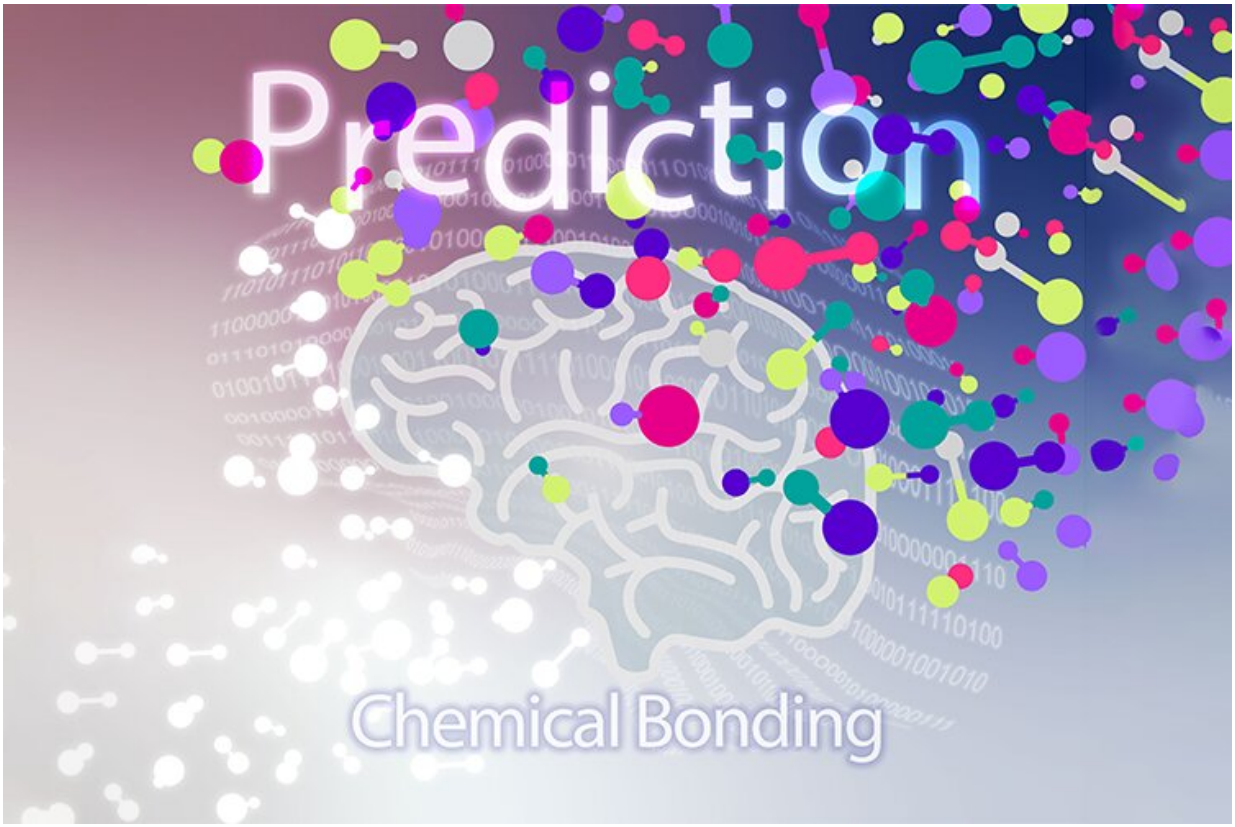

Researchers from The University of Tokyo Institute of Industrial Science report a machine learning-based model for predicting the bonding properties of materials. Credit: Institute of Industrial Science, the University of Tokyo

Designing materials that have the necessary properties to fulfill specific

functions is a challenge faced by researchers working in areas from catalysis to solar cells. To speed up development processes, modeling approaches can be used to predict information to guide refinements. Researchers from The University of Tokyo Institute of Industrial Science have developed a machine learning model to determine characteristics of bonded and adsorbed materials based on parameters of the individual components. Their findings are published in *Applied Physics Express*.

Factors such as the length and strength of bonds in materials play crucial roles in determining the structures and properties we experience on the macroscopic scale. The ability to easily predict these characteristics is therefore valuable when designing new materials.

The density of states (DOS) is a parameter that can be calculated for individual atoms, molecules, and materials. Put simply, it describes the options available to the electrons that arrange themselves in a material. A modeling approach that can take this information for selected components and produce useful data for the desired product—with no need to make and analyze the material—is an attractive tool.

The researchers used a machine learning approach—where the model refines its response without human intervention—to predict four different properties of products from the DOS information of the individual components. Although the DOS has been used as a descriptor to establish single parameters before, this is the first time multiple different properties have been predicted.

"We were able to quantitatively predict the binding energy, bond length, number of covalent electrons, and the Fermi energy after bonding for three different general types of system," explains study first author Eiki Suzuki. "And our predictions were very accurate across all of the properties."

Because the calculation of DOS of an isolated state is less complex than for bonded systems, the analysis is relatively efficient. In addition, the neural network model used performed well even when only 20% of the dataset was used for training.

"A significant advantage of our model is that it is general and can be applied to a wide variety of systems," study corresponding author Teruyasu Mizoguchi explains. "We believe that our findings could make a significant contribution to numerous development processes, for example in catalysis, and could be particularly useful in newer research areas such as nano clusters and nanowires."

The article, "Accurate Prediction of Bonding Properties by a Machine Learning-based Model using Isolated States Before Bonding", was published in *Applied Physics Express*.

More information: "Accurate Prediction of Bonding Properties by a Machine Learning-based Model using Isolated States Before Bonding", *Applied Physics Express*, DOI: 10.35848/1882-0786/ac083b

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