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Artificial Intelligence Algorithm & Laws of Quantum Mechanics

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Editorial

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EDITORIAL NOTE

The electronic characteristics of molecules and molecular wave functions can be predicted using artificial intelligence. A team of researchers from the University of Warwick, the Technical University of Berlin, and the University of Luxembourg discovered a novel AI technology that might be used to speed up the design of medicinal compounds or new materials. Artificial intelligence and machine learning algorithms are frequently employed to forecast our buying habits and recognize our faces or handwriting. Artificial Intelligence is establishing itself as a critical instrument for scientific discoveries in scientific study. In chemistry, artificial intelligence has proven to be useful in predicting the results of experiments or simulations of quantum systems. To accomplish this, AI must be able to incorporate the fundamental rules of physics in a systematic manner. Quantum computing is a new type of computing that is based on quantum mechanics. It carries out computations using quantum units under control. Quantum computers can only address problems that traditional computers can solve in terms of computable problems, but in terms of computing efficiency, some known quantum algorithms are tenfold quicker than traditional general-purpose computers due to the existence of quantum superposition.

Each neuron is set to a certain state before being developed to a steady state. One of the patterns in a training set is the output result. The simulation findings reveal that this network operates in a quantum environment and that the output images are correct, indicating that the protocol's viability has been established.

A deep machine learning algorithm developed by an interdisciplinary team of chemists, physicists, and computer scientists led by the University of Warwick and including the Technical University of Berlin and the University of Luxembourg can predict the quantum states of molecules, also known as wave functions, which determine all properties of molecules. Solving these equations in the traditional approach necessitates a large amount of high-performance computing resources (months of computing time), which is generally the bottleneck in the development of new purpose-built molecules for medicinal and industrial uses. On a laptop or smartphone, the newly built AI programme can provide correct forecasts in seconds.

"This has been a joint three-year effort, which required computer science know-how to develop an artificial intelligence algorithm flexible enough to capture the shape and behavior of wave functions, but also chemistry and physics know-how to process and represent quantum chemical data in a form that is manageable for the algorithm," says Dr. Reinhard Maurer of the University of Warwick's Department of Chemistry.

Prof. Dr. Klaus Robert-Muller of the Technical University of Berlin's Institute of Software Engineering and Theoretical Computer Science adds:

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"This interdisciplinary research is significant because it demonstrates that AI can efficiently conduct the most difficult portions of quantum molecule simulations. AI approaches will become an integral element of the discovery process in computational chemistry and molecular physics within the next few years."

Professor Dr. Alexandre Tkatchenko of the University of Luxembourg's Department of Physics and Materials Research concludes: "This study offers a new level of compound design in which both the electrical and structural properties of a molecule can be tweaked simultaneously to meet specific application criteria," says the researcher.