# A Machine Learning Algorithm for Material Property Predictions

**Using machine learning models to perform material simulations with quantum mechanics**

Inventors at Georgia Tech have developed a data-driven machine learning (ML) approach to solve the electronic structure problem. This new approach requires a critical amount of initial training data (obtained from reference quantum mechanics calculations) which are then used to train a ML algorithm. Once trained, the ML model can solve the electronic structure problem, i.e., yield the electronic charge and energy level arrangements, several orders of magnitude faster than the parent quantum mechanics calculations while preserving accuracy. Applications include any situation where a quantum mechanical simulation is required and situations when materials discovery has to be aided by computational quantum mechanics.

**Summary Bullets**

- **Faster:** this approach provides a speed up of several orders of magnitude relative to the current methods
- **Accuracy:** despite faster speed, accuracy is not compromised
- **Efficient:** solves electronic structure problems

Solution Advantages

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Potential Commercial Applications

- Creation of structural and functional materials meeting a target requirement
- Simulations of catalytic systems
- Energy storage materials

Background and More Information

Traditional experiments and computational modeling often consume tremendous amounts of time and have many experimental limitations. By using machine learning for the design and discovery of new materials, there is the possibility to achieve great improvements in both time and accuracy. Virtual material discovery using

computational quantum mechanics methods are accurate, but enormously time-intensive. Such methods solve the "electronic structure problem" first, which results in the electronic charge and energy level arrangements. These results are subsequently used to compute other useful material properties. The primary bottleneck in computational quantum mechanics based approaches is the solution of the electronic structure problem.

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**IP Status**

Patent application has been filed : US62/744593

**Publications**

Using Machine Learning to Create More Capable Capacitors, UC San Diego News(Wise) - June 26, 2019

**Images**

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