Yottaasys Develops AI Alternative to DFT for discovering New Crystals

Yottaasys Develops AI Alternative to DFT for discovering New Crystals.

INDIA, January 23, 2020 /EINPresswire.com/ -- This use case was implemented for one of the worlds leading semiconductor manufacturer.

Background:

Semiconductors materials such as silicon (Si), germanium (Ge) and gallium arsenide (GaAs), have electrical properties somewhere in the middle, between those of a “conductor” and an “insulator”. They are not good conductors nor good insulators (hence their name “semi”-conductors). They have very few “free electrons” because their atoms are closely grouped together in a crystalline pattern called a “crystal lattice” but electrons are still able to flow, but only under special conditions.

The ability of semiconductors to conduct electricity can be greatly improved by replacing or adding certain donor or acceptor atoms to this crystalline structure thereby, producing more free electrons than holes or vice versa. That is by adding a small percentage of another element to the base material, either silicon or germanium.

On their own Silicon and Germanium are classed as intrinsic semiconductors, that is they are chemically pure, containing nothing but semi-conductive material. But by controlling the amount of impurities added to this intrinsic semiconductor material it is possible to control its conductivity. Various impurities called donors or acceptors can be added to this intrinsic material to produce free electrons or holes respectively.

This process of adding donor or acceptor atoms to semiconductor atoms (the order of 1 impurity atom per 10 million (or more) atoms of the semiconductor) is called Doping. The as the doped silicon is no longer pure, these donor and acceptor atoms are collectively referred to as “impurities”, and by doping these silicon material with a sufficient number of impurities, we can turn it into an N-type or P-type semi-conductor material.

Objective:

Discovering a new Crystal structure (Alloy) for semi conductors is Highly Specialized and time-consuming task using tradition Material Sciences, At the very minimum there are 10 million possible recipes for any possible scenario. Further, the material needs both electrically conductive and have a low absorption in the visible range, which are typically competing properties.

The automated Machine Learning model eliminated the need of quantum-mechanical method known as density-functional theory (DFT). DFT calculations are expensive, requiring hundreds or thousands of CPU hours on supercomputers for large systems and prohibit the modelling of a sizeable number of possible compositions and configurations

Solution:

This was a multi target prediction problem and the two Target variables were

Formation energy: one of the most important properties of a compound that is directly related to its stability. More negative the formation energy, the more stable the compound is likely to be

Bandgap energy: It is the energy required to promote a valence electron bound to an atom to become a conduction electron, which is free to move within the crystal lattice and serve as a charge carrier to conduct electric current. It is closely related to the HOMO/LUMO gap in chemistry.

“The Team has been instrumental in creating an AI based alternative to DFT and the overall predictive analytics solution, it has helped us in reducing overall product design cycle time and reduce efforts”
Shenyuan wang, PHD DFT Analaysis, Client Team

Arun Pandey
Yottaasys
+91 80 4370 7012
email us here
Visit us on social media:
LinkedIn
