

Name:

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Class:

# Designing for Next-Generation Technology Reading

## What Is Density Functional Theory (DFT)

Imagine zooming way, way in, so close you can see the atoms that make up everything around you. Even smaller than atoms are electrons, the tiny particles that move around and create electricity, magnetism, and chemical bonds. Scientists want to know: How do these electrons behave? That is where Density Functional Theory (DFT) comes in.

**DFT** is a computer-based method that helps scientists predict how atoms and electrons interact without needing to do physical experiments. Instead of looking at every electron (which would take forever), DFT looks at the overall electron density, like a cloud showing where electrons are likely to be.

Using DFT, scientists can:

- Find out which materials conduct electricity or block it.
- Understand how strong or reactive a material is.
- Design new batteries, computer chips, and memory devices.

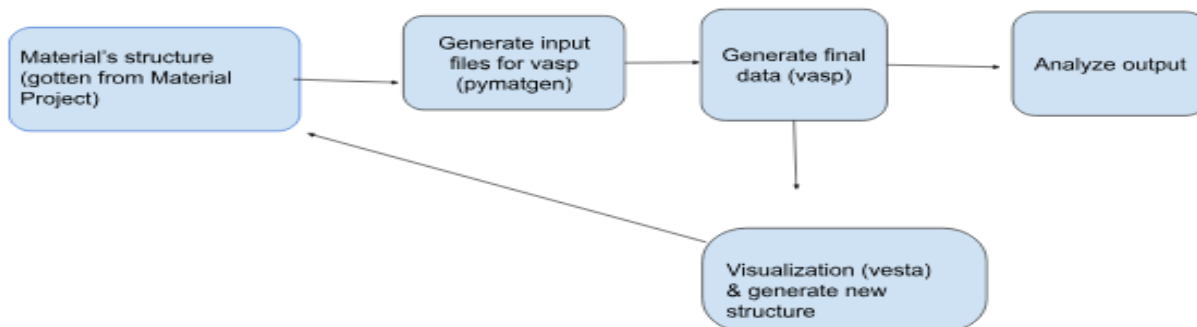
DFT is used by engineers, chemists, and physicists around the world to explore what happens inside materials at the atomic level—something you cannot see with your eyes. It is like having a microscope that uses math and physics to explore invisible worlds.

## Tools & Methodology

The main tools material science researchers use are:

- Pymatgen (generate files from structures of materials for VASP).
- Vienna ab-initio Simulation Package (VASP) (DFT codes; get final results for researchers).
- Visualization for Electronic and Structural Analysis (VESTA) (visualize the structures of materials).

## diagram of the process of computational engineering



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