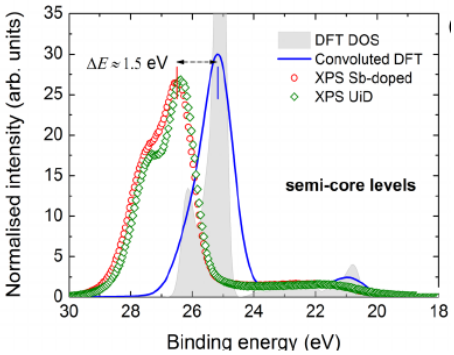
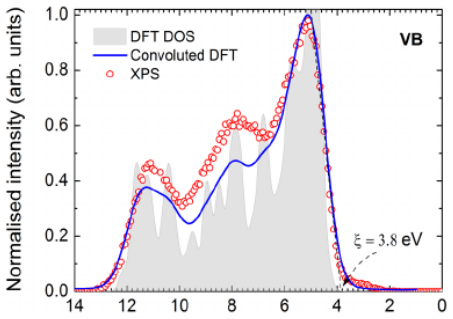
Density Functional Theory Calculation Service



Density functional theory (DFT) is a computational quantum mechanical modeling used in physics, chemistry, and materials science to evaluate the electronic structure (or nuclear structure, principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. A many-electron system's properties can be determined using functionals, i.e., functions of another function. In the case of DFT, these are functionals of the spatially dependent electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

Overall solutions



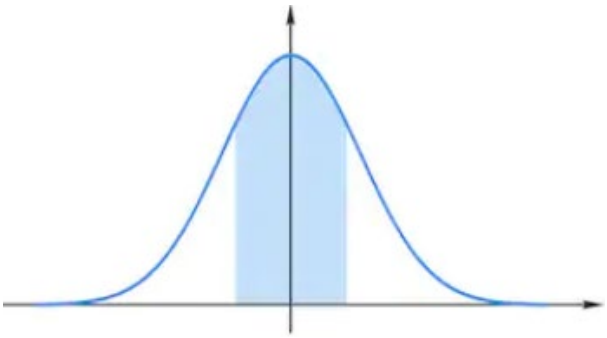
- The essence of density functional theory is to transform the wave function into an electron density function as the basic unit of research, thereby simplifying the calculation process, and converting the multi-electron problem into a single-electron problem for solution.
- Assuming that the number of electrons is N, the total number of variables in the wave function is 3N, and the solution is extremely complicated. Using density functional theory, the number of variables can be reduced to three, that is, only three spatial variables are included. Using DFT can simplify the calculation process, and ensure the calculation accuracy.

- Our bioinformaticians will provide the most accurate density functional theory calculation service for our clients.

Our services

Project name	Density Functional Theory Calculation Service
Samples requirement	Our density functional theory calculation service requires you to provide
Timeline	Decide according to your needs.
Deliverables	We provide you with raw data and analysis service.
Price	Inquiry

Applications



- Developing new functional materials in materials science, in particular nanotechnology.
- Studying the properties of fluids at a surface and the phenomena of wetting, adsorption.
- Understanding life processes in biotechnology.
- Improving filtration methods for gases and fluids in chemical engineering.
- Studying and identifying solutions for water and air pollution in environmental science.
- Generating new procedures in microfluidics and nanofluidics.

CD ComputaBio can provide you but not limited to:

- QM/MM computing service

- Molecular electrostatic potential (MEP) calculation
- Natural bond orbit analysis (NBO)

CD ComputaBio' density functional theory calculation service can reduce the cost of later experiments. The density functional theory calculation service is a personalized and customized innovative scientific research service. Before determining the corresponding analysis plan and price, each project needs to be evaluated. If you want to know more about service prices or technical details, please feel free to contact us.