A fast, precise & flexible DFT code for ab-initio atomistic simulation

BigDFT is a modern Density Functional Theory software for ab-initio atomistic simulation of challenging materials and biological systems. It offers calculations for periodic systems, surfaces, wires, or isolated molecules, and thanks to the available linear scaling approach, also very large systems containing thousands of atoms can be simulated. The outstanding properties of BigDFT come from its Daubechies wavelets basis set. Wavelets form a flexible, systematic and accurate basis set that allow for an adaptive mesh.

DFT

Density Functional Theory (DFT) is a computational quantum mechanical modelling method to investigate the electronic structure of matter. It is widely used in physics, chemistry and materials science, and is one of the most popular electronic structure methods thanks to its good compromise between accuracy and speed. DFT can be considered as a parameter-free approach as it only requires positions of the atoms that build up the system to simulate.

BigDFT is a versatile and flexible code for in-silico characterization of challenging materials and bio-systems

Large systems

The linear scaling approach of BigDFT enables DFT simulations for systems containing thousands of atoms.

Massively parallel

The multi-level parallelization of BigDFT allows the code to scale to thousands of cores and to run efficiently on the most powerful supercomputers

Outstanding precision

The usage of norm-conserving pseudopotentials and the systematic wavelets basis set guarantee precise and efficient calculations.

Python interface

The modern Python interface allows to perform calculations with BigDFT using an easy and intuitive API.

Who can benefit from this technology?

Any organization (chemical company, university, research center...) performing innovative research of materials and molecular systems at the nanoscale.

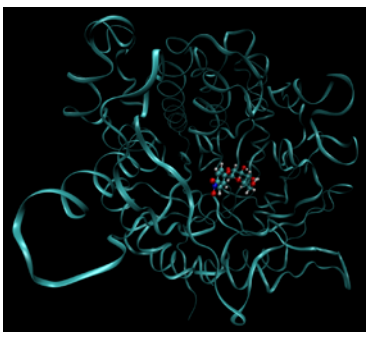
The unique features of BigDFT are well-suited for chemical applications such as

- Adsorption on surfaces and adhesion: corrosion inhibition, surface impregnation of dyes, wettability, rubber adhesion, adsorption of catalyzers.
- Heterogeneous catalysis: catalytic reaction, conformation of van-der-Waals complexes.
- Nanoclusters, oligomers, organic crystals, hypothetical MOFs, zeolite cages.
- OLEDs: electronic properties.
- Defects/Dopants in semiconductors, inorganic crystals or metals.

Platforms integrating BigDFT

NEXTMOL AiiDA

Use cases



Enzymes

Enzymes are proteins that promote chemical reactions, i.e. they act as biological catalysts and act upon substrates, which are the molecules that undergo the desired chemical reaction in the presence of the enzyme. An important property is the selectivity, i.e. the ability to act only on a specific substrate. BigDFT has been used to perform a full Quantum Mechanical calculation of a complex enzyme-substrate system and to identify those fragments of the enzyme that most interact with the substrate.

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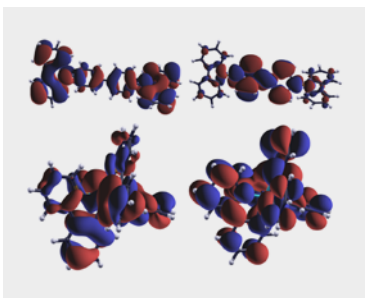
https://pubs.acs.org/doi/10.1021/acs.jctc.9b01152



OLEDs

BigDFT has been used to study a supramolecular structure that can be employed as organic light-emitting diode (OLED). The material was composed of a host transport matrix doped with optically active centers (guests), and the charge transport parameters were calculated on the basis of a CDFT method implemented in the linear-scaling approach of BigDFT.

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https://pubs.acs.org/doi/10.1021/acs.jctc.5b00057

For more information visit us here

www.bigdft.org