SIMULATE MATERIALS USING THE DENSITY FUNCTIONAL METHOD BY VASP SOFTWARE

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Abstract

There are many methods and software for simulating materials in practice today, each software or computational method has its own advantages and disadvantages. In the process of studying and researching material simulation, we found that the VASP software combined with the Density Functional Theory (DFT) method is perfect up to this point. Reliability, accuracy, and low resource and time consumption during the calculation process are the standout advantages of this combination. DFT calculations on VASP require the precise construction of input data, including the input files, and it is not necessary to write code to process the output data, which is a significant advantage compared to other methods. Output data is processed through commonly used support software such as Origin and VESTA, which is an advantage of this simulation calculation method.

Keywords: DFT method, DFT simulation, Materials simulation, VASP software

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1. Introduction

For modeling and computing the characteristics of semi-conductor materials, DFT is a strong and popular method (Jörg Neugebauer et al., 2013). DFT offers the following benefits when used to semiconductor materials: DFT can be used to precisely forecast the electronic band structure, electronic density of states, and other electronic properties of semiconductor materials (Mahmud et al., 2024).From small crystals to complex compounds, DFT can be used to simulate complicated material systems with many atoms (Ziheng Lu et al., 2022). Because DFT is more computationally efficient than other quantum theory techniques like the Full-potential approach or the Many-Body method, larger systems can be simulated faster (Lalith Perera et al., 2014). DFT offers a wide range of density functional types (including LDA, GGA, and hybrid functionals) that are appropriate for varied materials and applications, increasing flexibility in simulations (Aminul Islam et al., 2025). DFT not only simulates electronic properties well but also other properties such as magnetic, structural, dynamical, and optical properties of semiconductor materials (Nzar Rauf Abdullah et al., 2024).

There are many software and computational libraries that support DFT, such as VASP (Hafner et al., 2007), Quantum ESPRESSO (Paolo Giannozzi et al., 2009), and ABINIT

(Xavier Gonze et al., 2020), which help researchers easily apply and harness the power of DFT. DFT has become an important theoretical method and is widely used in the research and development of new semiconductor materials.

In this theory, the properties of the N-electron system are represented through the electron density function of the entire system (which is a function of 3 spatial coordinates) instead of the wave function (which is a function of 3N spatial coordinates).

The quantity of electrons in a unit volume is known as the electron density function. In general, the value of the electron density function will vary depending on the precise location in space. The number of electrons in this formulation must be interpreted probabilistically because electrons in quantum mechanics do not have definite coordinates. The spatial variables x, y, and z determine the electron density in this model

$$N = \int n(\vec{r})d\vec{r}. \tag{1}$$

The relationship between the electron density and the many-body wave function of the system is represented as follows:

$$n(\vec{r}) = N\int ...\int \left|\psi(\vec{x}_1, \vec{x}_2, ...\vec{x}_N)\right|^2 d\vec{x}_1, d\vec{x}_2, ..d\vec{x}_N. \tag{2}$$

Equation (2) displays the probability of finding any electron in the volume element $d\vec{r}$. By ensuring that the integral of the electron density across the entire space equals the total number of electrons in the system, N, the normalization criteria is satisfied. A point in space where the electron density is considered is represented by one of the spatial coordinate systems in this equation. The equation can be used to determine the energy functional of an interacting electron system moving in an external potential field:

$$V_{ext} = \int n(\vec{r})v(\vec{r})d\vec{r}. \tag{3}$$

However, the charge density function is the sole way to express this part in the equation explicitly. It is impossible to define the kinetic energy factor K_e in an explicit manner due to the derivative of the wave function. The localization, which is indicated by the positions of the electrons in the denominator, makes it challenging to combine the terms in the electronic-electronic interaction energy term V_{ee}. These limitations prevent a universal energy density functional expression. Given their relationship to electrons, it will be more practical to merge the phrases K_e and V_{ee} into one word and write it like this:

$$F(\psi_e) = K_e + V_{ee}. \tag{4}$$

The system's total energy is:

$$E_e = F(\psi_e) + V_{ee}(v, n). \tag{5}$$

The subsequent section will transform $F(\psi_e)$ a functional of the wave function, into a func-tional of the electron density F(n) in order to express the electronic energy in the system in terms of the electron density.

There is only one external potential that corresponds to an arbitrary electron density, which may be chosen thanks to the Hohenberg-Kohn theorems. Consequently, this electron density corresponds to the Hamiltonian and just one external potential. Thus, it will also be possible to determine the Hamil-tonian and all associated features in a unique way. The variational concept can also be used to obtain the least amount of energy. This is essentially the act of altering the electron density in order to minimize energy (Viraht Sahni et al., 2004).

At this point, DFT is still not applicable to calculations in the actual world because there has been no simplification. An electron system interacting with a moving potential in an external field requires the solution of the Schrödinger equation. The Kohn-Sham assumption essentially replaces one problem with another. Kohn and Sham recommended sending a letter between

$$F(n(\vec{r})) = K_{ks}(n(\vec{r})) + V_H(n(\vec{r})) + E_{xc}(n(\vec{r})), \qquad (6)$$

From (6) function, where the classical electrostatic $V_H = (n(\vec{r}))$ interaction potential between the electrons (Hartree potential) is represented by the kinetic energy functional for the non-interacting Kohn-Sham electron system with electron density $n(\vec{r})$; and the exchange-correlation energy, $E_{xc} = (n(\vec{r}))$ which is the component that fills in all the gaps when comparing the real system and the Kohn-Sham system (John Pople et al., 1992).

2. VASP software

A computer application called VASP (Vienna Ab Initio Simulation Packages) is used to simulate materials at the atomic level. Mike Payne of MIT was the original developer of VASP. Later, in 1989, Jurgen Hafner moved VASP to the University of Vienna in Austria. In VASP, Jurgen Furthmuller wrote the core program. Georg Kresse is now working on VASP. The creation of techniques frequently seen in molecular quantum chemistry for periodic systems is one of the recent additions to VASP. Because the crystal potentials are appropriately generated, electronic-electronic interactions are fully included, and magnetic configurations are taken into account in the calculations, the VASP software provides a dependable computational tool for the majority of condensed matter materials. Furthermore, the PAW (projector-augmented wave) pseudopotentials can describe the intrinsic electron-ion interactions. So far, VASP has been used by more than 1400 research groups under a license agreement with the University of Vienna (Guangyu Sun et al., 2003).

The term "Limited VASP" could refer to either licensing restrictions or the inherent limitations of the software. VASP is a commercial software, meaning that only licensed users can access and use it. Some institutions may have a limited license, restricting the number of users or computational resources available. Computational limitations also play a significant role; while VASP can handle large systems with hundreds or thousands of atoms, memory (RAM) and CPU/GPU resources become critical, especially for demanding calculations like GW, hybrid functionals (HSE06), and BSE, which often require over 100GB of RAM. Scaling performance depends on parallelization settings (NPAR, KPAR, LPLANE, NSIM) and the available number of CPU cores. Additionally, some functional limitations exist, such as the high computational cost of hybrid functionals (HSE, B3LYP, etc.), the need for parameter tuning in DFT+U, and the extreme memory demands of GW/BSE calculations. Convergence issues can also arise, particularly for strongly correlated systems, metallic systems, or fine k-point sampling requirements**,** which increase computational costs. Moreover, Pulay stress and relaxation challenges can lead to inaccurate lattice parameters if not properly managed. If you are referring to "Limited VASP" as a restricted version of the software, it likely means you are using a license with reduced capabilities.

3. Calculation method

The Density Functional Theory method, combined with the Vienna Ab-initio Simulation Package, is a powerful tool for simulating electronic, structural, and dynamical properties of materials. Below is a comprehensive guide to performing DFT calculations using VASP.

3.1. Prepare input data

Define the material system**, s**elect the material to be simulated: semiconductors, metals, 2D materials, 1D materials, surfaces, heterostructures, etc. After that, determine the appropriate unit cell or supercell dimensions**.** Prepare input files, VASP requires four essential input files:

POSCAR: Defines the atomic structure (atomic coordinates, lattice parameters, etc.); POTCAR: Contains pseudopotentials describing the interaction between nuclei and electrons;

KPOINTS: Specifies the k-point sampling grid in the Brillouin zone;

INCAR: Sets the computational parameters controlling the simulation.

3.2. Calculation Steps

Geometry Optimization (Relaxation), and Optimize atomic positions to reach an energy-minimized equilibrium state.

INCAR Settings for Relaxation: ISTART = 0; IBRION = 2 (Conjugate Gradient or Quasi-Newton optimization method); NSW = 100 (Maximum number of ionic steps); EDIFF = $1E^{-5}$ (Energy convergence criterion); Check forces on atoms (FORCES) and stress tensor (STRESS) to ensure stability.

Next to Self-Consistent Field (SCF) Energy Calculation. After geometry relaxation, perform total energy calculations using: INCAR Settings for SCF Calculation, chose ISTART = 1 (Start from relaxed geometry); ALGO = Fast (Use efficient electronic minimization algorithm); EDIFF = 1E-6 (Higher convergence accuracy).

Run VASP to compute the stable electronic state; Property Calculations, once the SCF calculation is complete, analyze various material properties:

Band Structure Calculation by modify KPOINTS for band path sampling; Add ICHARG = 11 in INCAR to use the charge density from SCF; Extract results from EIGENVAL, PROCAR**.**

Density of States (DOS) Calculation:

Use LORBIT = 11 to obtain atom- or orbital-resolved DOS; Analyze results from DOSCAR**.**

Optical Properties Calculation, Enable LOPTICS = .TRUE. to compute dielectric functions; Analyze results from vasprun.xml; Magnetic and Spin Properties, Set ISPIN = 2 for spin-polarized calculations and use LORBIT = 11 to extract magnetic moments.

Post-Processing and Visualization, after running VASP, post-processing is essential for interpreting results:

- Structural Visualization: Use VESTA, VMD, Ovito to visualize atomic structures;
- Band Structure & DOS Analysis: Utilize p4vasp, VASPKIT, SUMO, pymatgen to plot results; Compare with Experimental Data to validate computational results.

Key Considerations, choose appropriate pseudopotentials (POTCAR):

PAW-PBE, PAW-LDA. Ensure convergence of ENCUT and KPOINTS: the recommended value in POTCAR; KPOINTS: Test convergence with a Monkhorst-Pack grid. If convergence issues arise, Adjusting ALGO, EDIFF, LREAL; modifying IBRION, ISMEAR; Increasing the number of ionic steps (NSW) for relaxation.

4. Calculation results

4.1 Input files

In this project, we apply DFT methode for calculations with VASP software to specific input files as follows with 1D materials:

INCAR file:

```
ribbon
ISMEAR=1
SIGMA=0.05
RWIGS=1.500 0.370
ISIF=2
PREC=High
ISPIN=2
MAGMOM=24*1
NSW=400
IBRION=2
LWAVE=.FALSE.
LREAL=.TRUE.
EDIFF=1E-6
EDIFFG=-0.01
NPAR=1
NGX=240
NGY=240
NGZ=80
```

KPOINTS file:

```
pure
 0
G
 1 1 12
 0 0 0
```

POSCAR file:

```
armchair N6
1.0
       25.0976791382        0.0000000000        0.0000000000
        0.0000000000       23.9598770142        0.0000000000
        0.0000000000        0.0000000000        7.9057679176
   X    H
   12    4
Direct
     0.520000000       0.261872000       0.666666667
     0.520000000       0.357123000       0.166666667
     0.520000000       0.452374000       0.666666667
     0.520000000       0.547626000       0.166666667
     0.520000000       0.738128000       0.166666667
     0.480000000       0.261872000       0.333333333
     0.480000000       0.357123000       0.833333333
     0.480000000       0.642877000       0.333333333
     0.480000000       0.738128000       0.833333333
     0.520000000       0.642877000       0.666666667
     0.480000000       0.452374000       0.333333333
     0.480000000       0.547626000       0.833333333
     0.500000000       0.197011000       0.780159000
     0.500000000       0.197011000       0.219841000
     0.500000000       0.802989000       0.719841000
     0.500000000       0.802989000       0.280159000
```

POTCAR file:

```
PAW_PBE X 08Apr2002
   4.00000000000000
 parameters from PSCTR are:
   SHA256 =  fa972ea603024cb82d8554cfb4e3c683082552a2e54046a4c72c994edc589ce1 Sn/POTCAR
   COPYR  = (c) Copyright 08Apr2002 Georg Kresse
   COPYR  = This file is part of the software VASP. Any use, copying, and all other rights are
regulated by the VASP license agreement.
   COPYR  = If you do not have a valid VASP license, you may not use, copy or distribute this
file.
   VRHFIN =Sn: s^2p^2
   LEXCH  = PE
   EATOM  =    94.0860 eV,    6.9151 Ry
   TITEL  = PAW_PBE Sn 08Apr2002
   LULTRA =        F    use ultrasoft PP ?
   IUNSCR =        1    unscreen: 0-lin 1-nonlin 2-no
   RPACOR =    2.000    partial core radius
   POMASS =  118.710; ZVAL   =    4.000    mass and valenz
   RCORE  =    3.000    outmost cutoff radius
   RWIGS  =    2.960; RWIGS  =    1.5xx    wigner-seitz radius (au A)
   ENMAX  =  103.236;
   ENMIN  =   77.427 eV
   ICORE  =        3    local potential
   LCOR   =        T    correct aug charges
   LPAW   =        T    paw PP…
```

4.2 Data processing results

With the initial results prepared in POSCAR file, we can draw the material structure (Fig 1), through the parameters of name, position and size, connections of atoms in the unit cell, size of the unit cell in 3 dimensions and configuration characteristics, operating mechanism that allows (T) or does not allow (F) to move the position of atoms in the original crystal when calculating.

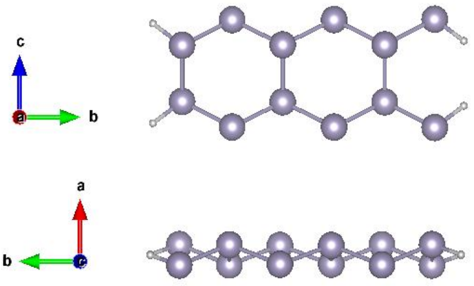

Fig 1. The POSCAR of AXNRs drawn with VESTA

Based on the output results of ORZICAR.dat and CONTCAR.dat files, we can extract data on the formation energy of the substance and magnetic field parameters, charge density parameters through orbitals, and spin quantum data through orbitals.

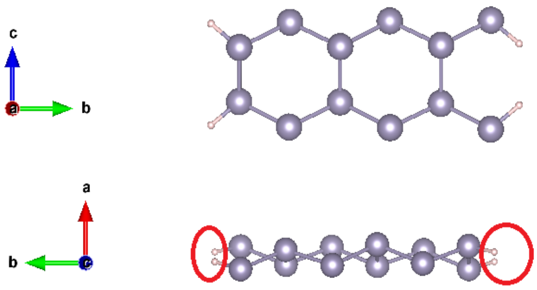

Fig 2. The CONTCAR of AXNRs drawn with VESTA

TABLE 1. Result calculation of AXNRs by VASP

E_P (eV)	-45.45
E_X (eV)	x
E_{X+P} (eV)	x
ΔE (eV)	x
Buckl (Å)	1.00
X-X (Å)	2.82
X-Pb (Å)	x
Deg	108.05
Mag (μ_B)	0.00
Eg (eV)	0.26

After calculating on VASP and processing data on Origin, we draw the results of the BAND energy band structure, PDOS state density, and electron density of the AXNRs structure presented in the figures.With the output data from the vasprun.xml file, we extracted the Xdos.dat and XBand.dat files and drew the BAND and DOS images using Origin software.

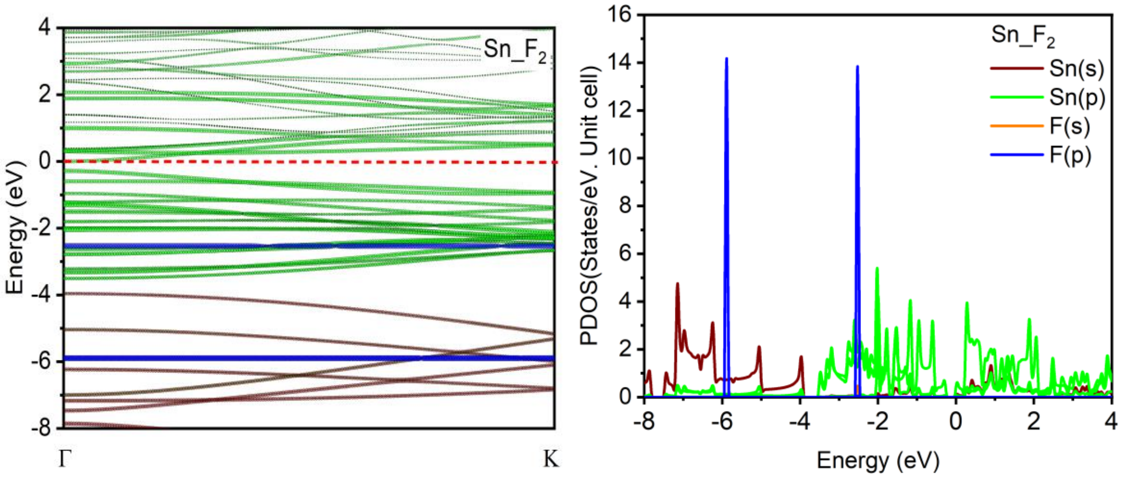

Fig 3. The BAND, PDOS of ASnNRs adsorbed F_2 drawn with Origin

From the CHGCAR output data file, we proceed to draw the electron density through the VESTA software after a few steps. With this drawing step, we choose the charge density from level (-) to level (+) corresponding to a certain value range that then corresponds to the GBR color range (Green, Blue and Red). If the result is red, it means that this area of space is losing (giving away) electron charges and conversely, this area is blue, it can be understood that this area is having a lot of electron charges (regaining).

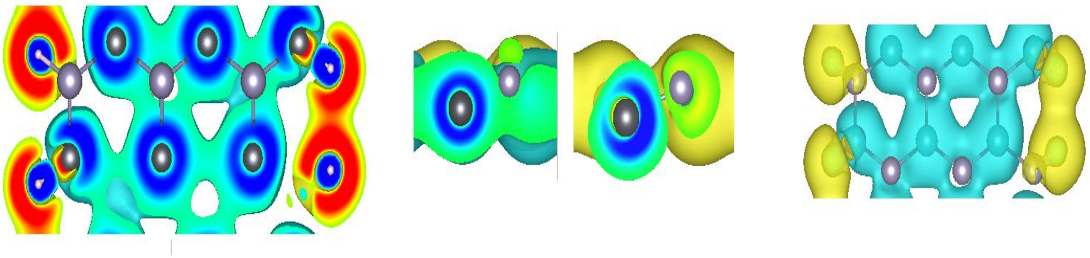

Fig 4. The charge density of XNRs drawn with VESTA

5. Conclustion

Through the process of research and direct calculation on VASP software to simulate materials using the DFT method, we see that this is an effective and easy-to-use calculation method. Because the (pseudo-potential) functions here have been included in the software by the suppliers during the calculation process, just need to declare the initial conditions, the functions will receive commands and execute. However, it is important that users know how to properly use the necessary functions, suitable for the materials and conditions being studied so that the calculation results are correct and optimal.

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