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# Overview of the VASP Software and Its Applications in Materials Research


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**ABSTRACT:** The rapid advancement of computational materials science has significantly accelerated the discovery and design of advanced materials at the atomic scale. Among the various first-principles simulation packages, the Vienna Ab initio Simulation Package (VASP) has become one of the most powerful and widely used computational tools in modern materials research. This review presents a comprehensive overview of the theoretical foundations, main functionalities, and applications of VASP in computational materials science. The fundamental principles underlying VASP, including Density Functional Theory (DFT), plane-wave basis sets, and the Projector Augmented Wave (PAW) method, are discussed in detail. In addition, the major computational capabilities of VASP, such as geometry optimization, electronic structure calculations, magnetic property analysis, optical property simulations, and ab initio molecular dynamics (AIMD), are systematically summarized. Particular attention is devoted to the applications of VASP in the investigation of two-dimensional materials, semiconductors, catalytic systems, gas adsorption, and energy-related materials, including lithium-ion batteries, photocatalysts, and perovskite solar cells. The advantages and current limitations of VASP are also analyzed, together with recent development trends involving machine learning, high-throughput calculations, workflow automation, and AI-assisted materials discovery. Owing to its high computational accuracy, scalability on high-performance computing platforms, and extensive methodological support, VASP continues to play a crucial role in advancing modern computational materials research and the development of next-generation functional materials.



**KEYWORDS:** VASP; Density Functional Theory; First-principles calculations; Electronic properties; Two-dimensional materials; Computational materials science


## I. INTRODUCTION

Over the past few decades, the rapid advancement of computational materials science has enabled the investigation and design of novel materials at the atomic scale prior to experimental realization. Among the most prominent and widely employed simulation tools is the VASP (Vienna Ab initio Simulation Package), a quantum-mechanical software package based on first-principles calculations. VASP was developed by Georg Kresse and co-workers at the University of Vienna for studying electronic structures, material properties, and ab initio molecular dynamics of condensed matter systems [1-2]. The software is primarily based on Density Functional Theory (DFT), employing plane-wave basis sets in combination with the Projector Augmented Wave (PAW) method [3-4]. Owing to its high computational accuracy, excellent optimization for high- performance computing (HPC) systems, and support for advanced approaches such as DFT+U, hybrid functionals, GW approximation, and ab initio molecular dynamics (AIMD), VASP has become one of the leading computational tools in the fields of nanomaterials, semiconductors, catalysis, magnetic materials, and energy-related materials research [5-6].

## 2. DEVELOPMENT HISTORY OF VASP

VASP was originally developed in the early 1990s based on the pioneering work of Georg Kresse and Jürgen Furthmüller in the field of first-principles electronic structure calculations [7]. The software was initially designed to efficiently solve electronic structure


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problems in solid-state materials using Density Functional Theory (DFT) in combination with plane-wave basis sets [8]. Early developments of VASP primarily focused on improving iterative diagonalization algorithms and optimizing computational performance for periodic systems, thereby enabling accurate and efficient total-energy calculations for crystalline materials. These advancements significantly contributed to the widespread adoption of VASP in computational condensed matter physics and materials science, particularly for large-scale simulations on high-performance computing platforms [9].

## 3. THEORETICAL FOUNDATIONS OF VASP

### 3.1. Density Functional Theory (DFT)

The theoretical framework of VASP is primarily based on Density Functional Theory (DFT), which is one of the most widely used quantum-mechanical approaches for investigating the electronic properties of condensed matter systems. DFT provides an efficient method for determining the ground-state properties of many-electron systems by describing the system in terms of electron density rather than many-body wave functions. The fundamental basis of DFT originates from the Hohenberg–Kohn theorems and the Kohn–Sham formalism [10-11], which established the theoretical foundation for modern first-principles electronic structure calculations. Due to its balance between computational efficiency and accuracy, DFT has become an essential tool in computational materials science, enabling the investigation of structural, electronic, magnetic, and optical properties of a wide variety of materials systems [12].

### 3.2. Plane-Wave Basis Set Method

VASP is primarily based on Density Functional Theory (DFT), a quantum-mechanical framework that enables the determination of the ground-state properties of many-electron systems using the electron density rather than the many-body wave function. The theoretical foundation of DFT was established through the seminal Hohenberg–Kohn theorems [13] and the Kohn–Sham formalism [14], which transformed modern computational materials science by providing an efficient approach for solving interacting electron systems. The Kohn–Sham equation is expressed as Eq.(1):

$$[-\frac{\hbar^2}{2m}\nabla^2 + V_{eff}(\vec{r})]\Psi_i(\vec{r}) = \varepsilon_i\Psi_i(\vec{r}) \qquad (1)$$

where $V_{ext}$ denotes the external potential, $V_H$ represents the Hartree potential, $V_{xc}$ corresponds to the exchange–correlation potential, and $\Psi_i(\vec{r})$ refers to the Kohn–Sham orbitals. Based on this formalism, DFT provides an accurate and computationally efficient framework for investigating a broad range of material properties, including electronic band structures, density of states (DOS), charge density distributions, magnetic moments, adsorption energies, and optical properties. Consequently, DFT-based calculations implemented in VASP have become indispensable in contemporary studies of nanomaterials, semiconductors, catalytic systems, magnetic materials, and energy-related materials [15-16].

### 3.3. Projector Augmented Wave (PAW) Method

The Projector Augmented Wave (PAW) method employed in VASP significantly improves the accuracy of first-principles calculations by providing a more precise description of the interactions between core and valence electrons. Compared with conventional pseudopotential approaches, the PAW formalism combines the computational efficiency of pseudopotentials with the accuracy of all-electron methods, making it one of the major advantages of VASP in achieving highly reliable electronic structure calculations for a wide variety of materials systems [15].

## 4. MAIN FUNCTIONS OF VASP

### 4.1. Geometry Optimization

VASP enables accurate structural optimization of various materials systems, including lattice constants, atomic positions, crystal geometries, two-dimensional (2D) materials, and low- dimensional nanostructures through efficient total-energy minimization and force calculations. Owing to its robust implementation of Density Functional Theory (DFT) and the Projector Augmented Wave (PAW) method, VASP has become one of the most widely used computational tools for investigating the structural stability and electronic properties of emerging nanomaterials. In recent years, VASP has been extensively applied in the study of 2D materials and nanoscale systems such as stanene, graphene, silicene, germanene, MXenes, and various nanoribbon structures, where first-principles calculations play a crucial role in understanding their electronic, magnetic, optical, and adsorption properties [17-20].

### 4.2. Electronic Properties

VASP is capable of calculating a wide range of electronic properties, including electronic band structures, density of states (DOS), projected density of states (PDOS), charge density distributions, electron localization functions (ELF), and work functions, which are

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essential for understanding the electronic behavior of materials at the atomic scale. Owing to its accurate implementation of Density Functional Theory (DFT) and plane-wave-based approaches, VASP has been extensively employed to investigate the electronic characteristics of low-dimensional nanostructures and emerging two-dimensional materials. In particular, for gas adsorption studies on stanene nanoribbons, VASP calculations have been widely used to analyze the variations in band gap and Fermi level induced by adsorbed gas molecules, thereby providing important insights into sensing performance, charge transfer mechanisms, and adsorption-induced electronic modifications [21-23].

### 4.3. Magnetic Properties

Through spin-polarized calculations, VASP provides an effective framework for investigating magnetic properties in condensed matter systems, including ferromagnetism, antiferromagnetism, half-metallicity, and spintronic behavior. By incorporating spin-dependent electronic interactions within the Density Functional Theory (DFT) formalism, VASP enables accurate evaluation of magnetic moments, spin polarization, exchange interactions, and magnetic stability in a wide variety of materials systems. In recent years, numerous first-principles studies have employed VASP to explore the effects of transition-metal doping, particularly Fe, Co, and Mn atoms, in two- dimensional materials and nanostructures. Such investigations have demonstrated that transition- metal dopants can significantly modify the electronic and magnetic properties of 2D systems, leading to induced magnetism, enhanced spin polarization, and potential applications in next- generation spintronic devices [24-26].

### 4.4. Optical Properties

VASP is capable of calculating a variety of optical properties, including the dielectric function, absorption coefficient, refractive index, reflectivity, and electron energy-loss spectra (EELS), which are essential for understanding light–matter interactions in materials systems. Based on Density Functional Theory (DFT) and frequency-dependent linear response theory, the optical properties module implemented in VASP enables detailed investigations of the electronic excitation behavior and optical responses of solids, nanostructures, and low-dimensional materials. Consequently, VASP has been widely employed in studies of optoelectronic materials, photovoltaic systems, photocatalysts, and optical sensing materials, where accurate prediction of optical spectra is crucial for evaluating device performance and electronic transitions [27-28].

### 4.5. Ab Initio Molecular Dynamics (AIMD)

VASP supports ab initio molecular dynamics (AIMD) simulations based on Density Functional Theory (DFT), enabling the investigation of finite-temperature behaviors and dynamic processes in materials systems at the atomic scale. Through AIMD calculations, VASP can be employed to study thermal stability, phase transitions, atomic diffusion, and surface interactions with high accuracy by explicitly considering the evolution of atomic configurations over time. Owing to these capabilities, AIMD simulations implemented in VASP have been extensively utilized in the study of nanomaterials, catalytic surfaces, battery materials, and low-dimensional systems, where temperature-dependent structural stability and atomic migration play crucial roles in determining material performance and functionality [29-30].

## 5. APPLICATIONS OF VASP IN MATERIALS SCIENCE RESEARCH

### 5.1. Research on Two-Dimensional Materials

VASP has been extensively employed in the investigation of two-dimensional (2D) materials, including graphene, silicene, germanene, stanene, phosphorene, and MXenes, owing to its high accuracy in describing the electronic and structural properties of low-dimensional systems. First- principles calculations performed using VASP have played a crucial role in understanding the fundamental physics and potential technological applications of these emerging nanomaterials. In particular, numerous studies have focused on band-gap engineering, gas adsorption behavior, atomic doping, and spin–orbit coupling effects, which are essential for tailoring the electronic, magnetic, optical, and transport properties of 2D materials for applications in nanoelectronics, sensing devices, catalysis, and spintronics. The incorporation of spin–orbit coupling within VASP is especially important for heavy-element-based 2D systems such as stanene and germanene, where relativistic effects strongly influence the electronic band structure and topological properties [31-34].

### 5.2. Semiconductor Materials Research

VASP has been widely utilized in semiconductor materials research due to its capability to accurately investigate electronic band structures, donor and acceptor levels, charge transport characteristics, and doping effects in a broad range of materials systems. Based on Density Functional Theory (DFT), VASP enables detailed analysis of the electronic properties of semiconductors at the atomic scale, thereby providing valuable insights into the relationship between atomic configurations and electronic behavior. In particular,

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the incorporation of hybrid exchange–correlation functionals, such as the Heyd–Scuseria–Ernzerhof (HSE06) functional, significantly improves the accuracy of calculated band gaps compared with conventional local or semi-local approximations, making VASP a highly reliable tool for predicting the electronic properties of semiconductors and optoelectronic materials. The HSE06 functional has therefore become extensively adopted in first-principles studies of doped semiconductors, defect engineering, and band-gap tuning in emerging nanomaterials [35-38].

### 5.3. Catalysis and Gas Adsorption Studies

VASP has been extensively applied in studies of catalysis and gas adsorption, particularly in research related to hydrogen evolution reactions (HER), oxygen evolution reactions (OER), lithium-ion battery materials, gas sensors, and molecular adsorption processes. Owing to its accurate implementation of Density Functional Theory (DFT), VASP enables detailed investigations of adsorption mechanisms, surface reactivity, charge transfer processes, and catalytic activity at the atomic scale. The adsorption energy, which is a key parameter for evaluating the interaction strength between adsorbates and material surfaces, is commonly calculated using

$$E_{ads} = E_{system} - E_{surface} - E_{gas} \quad (2)$$

where $E_{system}$, $E_{surface}$, and $E_{gas}$ represent the total energies of the adsorption system, pristine surface, and isolated gas molecule, respectively. Based on adsorption energies, charge transfer analyses, and density of states (DOS) calculations, the sensing performance and catalytic activity of materials can be systematically evaluated. In recent years, these approaches have been widely employed to investigate low-dimensional materials, transition-metal-based catalysts, and nanostructured systems for energy conversion, gas sensing, and electrochemical applications [39- 42].

### 5.4. Energy Materials

VASP has become an essential computational tool in the investigation and design of advanced energy materials, owing to its high accuracy in predicting structural stability, electronic properties, ion diffusion behavior, and interfacial interactions at the atomic scale. First-principles calculations performed using VASP have been extensively applied in studies of lithium-ion batteries, sodium- ion batteries, supercapacitors, photocatalytic materials, and perovskite solar cells. In battery- related research, VASP is widely employed to analyze ion adsorption, diffusion pathways, charge transfer, and electrochemical performance of electrode materials. For supercapacitor and photocatalytic systems, VASP calculations provide valuable insights into electronic conductivity, optical absorption, and catalytic activity. Furthermore, in perovskite solar cells, VASP has played a crucial role in understanding band alignment, defect formation, carrier transport, and light- harvesting mechanisms, thereby contributing significantly to the development of high-efficiency energy conversion technologies [43-47].

## 6. ADVANTAGES OF VASP

VASP possesses several significant advantages that have made it one of the most widely adopted first-principles simulation packages in computational materials science. Owing to its robust implementation of Density Functional Theory (DFT), plane-wave basis sets, and the Projector Augmented Wave (PAW) method, VASP provides highly accurate predictions of structural, electronic, magnetic, and optical properties for a broad range of materials systems. In addition, the software is highly optimized for high-performance computing (HPC) environments, enabling efficient large-scale parallel calculations on modern supercomputers. VASP also supports numerous advanced computational approaches, including DFT+U, hybrid functionals, spin–orbit coupling, GW approximation, and ab initio molecular dynamics (AIMD), which considerably extend its applicability in modern materials research.

Another important advantage of VASP is its extensive international research community and long- standing scientific reliability. The software has been extensively validated and continuously developed over several decades, resulting in highly reproducible and trustworthy simulation results. Furthermore, VASP is particularly powerful for periodic systems such as bulk crystals, surfaces, interfaces, two-dimensional materials, and nanostructures. Due to its computational accuracy and versatility, VASP has become one of the most frequently used simulation tools in high-impact scientific publications, especially in journals such as Physical Review B, Applied Surface Science, The Journal of Physical Chemistry C, Computational Materials Science, and Materials Today Physics [48-49].

## 7. LIMITATIONS OF VASP

Despite its numerous advantages and widespread applications in computational materials science, VASP still possesses several limitations. First, VASP is a commercial software package that requires a relatively expensive licensing fee, which may restrict accessibility for some research groups and institutions. In addition, due to the computational complexity of first-principles calculations

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based on Density Functional Theory (DFT), VASP generally demands substantial computational resources, particularly for large-scale systems, hybrid functional calculations, or ab initio molecular dynamics simulations performed on high-performance computing (HPC) platforms. Another limitation is that the software can be challenging for beginners because accurate simulations require careful selection of computational parameters, pseudopotentials, convergence criteria, and exchange–correlation functionals. Furthermore, conventional DFT approaches implemented in VASP may not accurately describe strongly correlated electron systems, such as transition-metal oxides and rare-earth compounds, where advanced methods including DFT+U, hybrid functionals, GW approximation, or beyond-DFT approaches are often necessary to achieve reliable results [50-51].

## 8. DEVELOPMENT TRENDS OF VASP

Recent developments of VASP have increasingly focused on improving computational efficiency, automation, and integration with data-driven materials science approaches. Modern versions of VASP are progressively incorporating advanced methodologies such as machine-learning interatomic potentials, high-throughput calculations, automated workflow management, and more efficient implementations of many-body approaches including the GW approximation and Random Phase Approximation (RPA). These developments significantly enhance the capability of VASP for large-scale materials discovery and accelerate the prediction of material properties with higher accuracy and lower computational cost. Furthermore, the integration of artificial intelligence (AI), data mining techniques, and materials informatics has positioned VASP as a central computational engine in next-generation computational materials research.

In parallel, a broad ecosystem of open-source platforms and workflow frameworks has been developed to directly support VASP calculations and large-scale automated simulations. Widely used tools such as pymatgen, ASE (Atomic Simulation Environment), VASPKIT, Materials Project, and Atomate provide efficient interfaces for structure generation, workflow automation, data analysis, high-throughput screening, and database construction. These platforms have greatly expanded the applicability of VASP in computational nanoscience, energy materials, catalysis, and AI-assisted materials discovery [52-56].

## 9. CONCLUSION

VASP has become one of the most powerful and widely utilized computational packages in the field of computational materials science. Based on Density Functional Theory (DFT) in combination with plane-wave basis sets and the Projector Augmented Wave (PAW) method, VASP enables accurate investigations of structural, electronic, magnetic, optical, and adsorption properties of a broad range of advanced materials systems. Owing to its high computational accuracy, excellent scalability on high-performance computing (HPC) platforms, and support for numerous advanced methodologies such as DFT+U, hybrid functionals, spin–orbit coupling, GW approximation, and ab initio molecular dynamics (AIMD), VASP has become an indispensable tool in modern research on nanomaterials, semiconductors, catalysis, and next-generation energy materials. Furthermore, the continuous integration of automated workflows, high-throughput calculations, and artificial intelligence-assisted materials discovery is expected to further strengthen the role of VASP in future computational materials research.

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