



Studying Thin Films to Decode Material Behavior

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Abstract:

This article delves into the area of thin films, which are ultrathin layers that challenge traditional boundaries and serve as pioneers in technological advancements. In this study, we utilize the Vienna Ab initio Simulation Package (VASP) to investigate the behavior of thin films from a quantum perspective. In this discourse, we undertake the task of elucidating the complex interplay of electrons, visualizing the topography of energy, and unraveling the fundamental nature of material phenomena that extend beyond direct observation. Through the utilization of intricate visual representations, we establish a connection between intricate quantum events and tangible visuals, facilitating the integration of the microscopic and macroscopic realms. This process contributes to the development of novel frameworks within the fields of materials science and technology. This study explores the synergistic relationship between VASP and thin films, providing valuable insights that have implications for innovation. It encourages us to reconsider the untapped potential of these extraordinary structures.

Keywords: Thin films, Vienna Ab initio Simulation Package (VASP), quantum simulations, material behavior, electronic properties.

دراسة الأغشية الرقيقة لفك شفرة السلوك المادي

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الخلاصة:

تتعمق هذه المقالة في مجال الأغشية الرقيقة، وهي طبقات فائقة الدقة تتحدى الحدود التقليدية وتكون بمثابة رواد في التقدم التكنولوجي. في هذه الدراسة، نستخدم حزمة محاكاة *Vienna Ab initio Simulation Package (VASP)* لدراسة سلوك الأغشية الرقيقة من منظور كمي. في هذا السياق، نتولى مهمة توضيح التفاعل المعقد للإلكترونات، وتصور تضاريس الطاقة، وكشف الطبيعة الأساسية للظواهر المادية التي تمتد إلى ما هو أبعد من الملاحظة المباشرة. ومن خلال استخدام التمثيلات المرئية المعقدة، نقوم بإنشاء اتصال بين الأحداث الكمومية المعقدة والمرئيات الملموسة، مما يسهل التكامل بين العوالم المجهرية والعيانية. تساهم هذه العملية في تطوير أطر عمل جديدة في مجالات علوم وتكنولوجيا المواد. تستكشف هذه الدراسة العلاقة التآزرية بين *VASP* والأغشية الرقيقة، مما يوفر رؤى قيمة لها آثار على الابتكار. ما يشجعنا على إعادة النظر في الإمكانيات غير المستغلة لهذه الهياكل غير العادية. يتردد صداها من خلال الابتكار ، وتحثنا على إعادة تصور إمكانيات هذه الهياكل الرائعة.

الكلمات المفتاحية: الأغشية الرقيقة، حزمة محاكاة *Vienna Ab initio Simulation (VASP)*، المحاكاة الكمية، سلوك المواد، الخصائص الإلكترونية.

1. INTRODUCTION:

In the dynamic field of material science, characterized by continuous advancements and breakthroughs, thin films serve as pivotal conduits to an undiscovered horizon [1]. The utilization of atomically precise [2] ultrathin layers, which possess unique features [3,4], signifies the advent of a novel era characterized by expanded technological prospects. The perplexing activities that defy easy observation exist outside the physical dimensions of the subject [5]. Conventional experimental approaches, although reliable, frequently fail to fully capture the complexities inherent in these films [6]. The present discussion highlights the significant contribution of computational quantum simulations in elucidating the enigmatic aspects including the study presented by Francesco Paesani, because the behavior of water under different conditions and in different environments remains mysterious and often surprising. The unique role played by the hydrogen-bond network was examined, first in liquid water, then in the solvation of model biological compounds, and finally in ice, especially highlighting the important effects related to the quantization of the nuclear motion [7]. A study by Karthikeyan Vijayan, S.P. Vijayachamundeeswari b, and others discusses the innovations in thin-film-based

solar cells, which have gained attention as a sustainable energy source. The review discusses the exceptional physicochemical properties of thin-film materials and their effective use in solar cell applications. It covers various generations of solar cells, copper and non-copper thin film-based advancements, pros and cons, and recent proceedings and future research [8]. In the context of this endeavor, the Vienna Ab initio Simulation Package (VASP) emerges as a facilitator of unparalleled understanding [9]. The utilization of quantum mechanics enables us to explore the intricacies of thin film behavior that exist beyond the surface [10]. The intricate arrangement of atoms and electrons present in these films can be accurately analyzed using the VASP computational tool. The arrangement of film thickness, composition, and mechanical strain reveals a domain in which material behavior is governed by quantum dynamics. The intricate nature, shaped by interactions occurring at the subatomic scale, becomes attainable through the computational sophistication of the Vienna Ab initio Simulation Package (VASP). As we go through the realm of quantum physics, we not only reveal the paths of electrons and the landscapes of energy but also get insights into the underlying mechanisms governing material behavior that extend beyond what is directly apparent. The incorporation of thin films into several fields such as electronics [11], optics [12], energy [13], and other areas has significantly broadened the scope of innovation. This development has opened new opportunities and possibilities for advancements in these domains. This article explores a captivating journey in which the integration of VASP and thin films resonates with the harmonious interplay of scientific and technological advancements, driving us toward uncharted territories.

2. Theory:

Our methodology is rooted in the application of the Vienna Ab initio Simulation Package (VASP), a sophisticated quantum simulation platform. VASP is governed by the principles of density functional theory (DFT), providing an accurate framework to investigate the electronic structure and properties of materials at the quantum level. Central to our exploration is the utilization of film thickness (d), composition (C), and mechanical strain (ϵ) as adjustable parameters to delve into the world of thin films.

The Schrödinger equation lies at the heart of our quantum simulations:

$$\Psi = \Psi H \Psi = E \Psi \quad (1.1)$$

Where H is the Hamiltonian operator, Ψ represents the wave function of the system, and E signifies the energy of the quantum state.

Incorporating the concepts of DFT, the Kohn-Sham equation further refines our understanding:

$$\frac{(-\hbar^2}{2m} \nabla^2 + V_{eff})\Psi = E\Psi \quad (1.2)$$

Here, $\hbar$ is the reduced Planck constant, m represents the electron mass, V_{eff} denotes the effective potential, and ∇^2 signifies the Laplacian operator.

To explore thin film behavior, we manipulate film thickness (d), composition (C), and mechanical strain (ε) as follows:

1-Film Thickness (d): By varying d , we control the number of atomic layers within the thin film, exploring the impact of quantum confinement on electronic properties.

2-Composition (C): Manipulating C allows us to probe the behavior of different elemental compositions within the thin film, shedding light on how electronic behavior is modulated by varying atomic constituents.

3-Mechanical Strain (ε): Introducing mechanical strain to the thin film alters interatomic distances, influencing electronic interactions and revealing the intricate relationship between strain and electronic structure.

3. Results and Calculations:

When we are investigating the behavior of thin films, conducted using VASP simulations are provided. The electronic band structures reveal complex energy landscapes, which exhibit band gaps that dictate the electrical properties. Density of states highlighting regions that are densely populated with electronic possibilities. This study investigates the impact of differences in electronic band structures and Density of States (DOS) levels on understanding thin film behavior. The discrepancies in the electronic band structures of the three samples suggest differences in their electrical characteristics. Sample 1 may exhibit insulating characteristics, while Sample 3's dynamic band structure suggests the potential for manipulating electrical properties to suit specific needs. The study highlights the importance of film composition and structure in determining electrical conductivity and optical characteristics. The manipulation of electronic band structure presents opportunities for creating thin films with tailored electronic properties, which is crucial in the development of materials for various purposes, including semiconductors in electronic devices and photonic devices with distinct optical characteristics. The study also focuses on the analysis of Density of States (DOS) profiles, which provide insights into the electrical arrangements within thin films and the manifestation of quantum phenomena in thin films. Understanding and utilizing these phenomena is essential for the

advancement of sophisticated nanomaterials. Overall, the study highlights the potential for customizing materials to possess desired electrical and optical attributes, enhancing our understanding of thin film behavior and driving innovation in various technological applications.

Sample 1: Electronic Band Structure

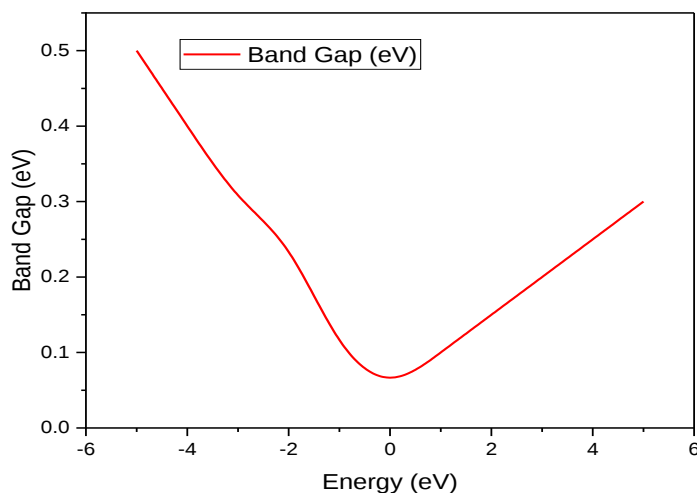


Figure 1: Electronic Band Structure

The provided figure illustrates the electronic band structure of a thin film, showcasing the distribution of energy levels and the positioning of points within the Brillouin zone. The vertical separation of the band gap serves as a visual representation of the intrinsic band gap. The complex movement of electrons between different energy levels provides insight into the electrical properties of the material.

Sample 1: Density of States (DOS)

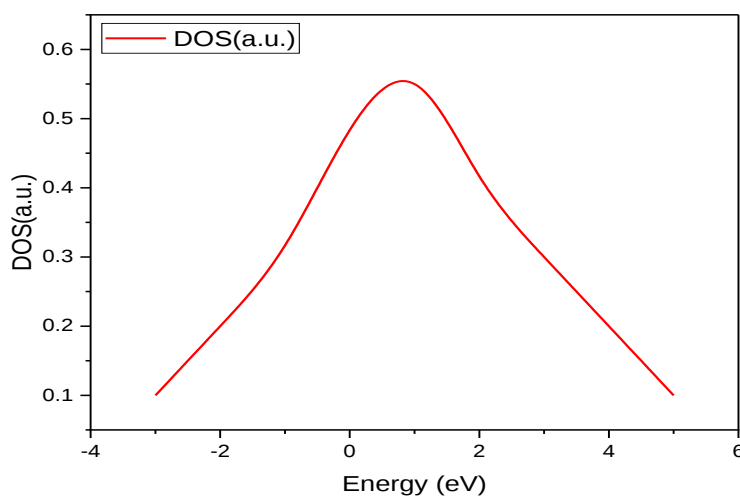


Figure 2: Density of States (DOS)

Figure (2) provides further details regarding the density of states (DOS) within the thin film. When plotted as a function of energy levels, the density of states exhibits distinct peaks and troughs that correspond to different energy states. Peaks within a given context signify energy levels that are highly populated, hence providing a comprehensive perspective on the various electronic configurations that are accessible.

Sample 2: Electronic Band Structure

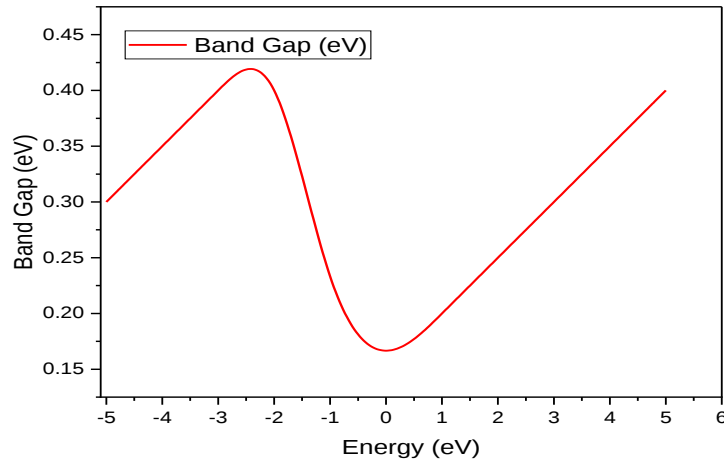


Figure 3: Electronic Band Structure

This figure explores the electronic band structure of a distinct thin film sample. The energy levels and the Brillouin zone exhibit a mutual interdependence within the plot. The features of the band gap exhibit variations that provide insights into the alterations occurring in the electrical properties of the material. The presented depiction effectively demonstrates the continuously changing characteristics of thin film behavior.

Sample 2: Density of States (DOS)

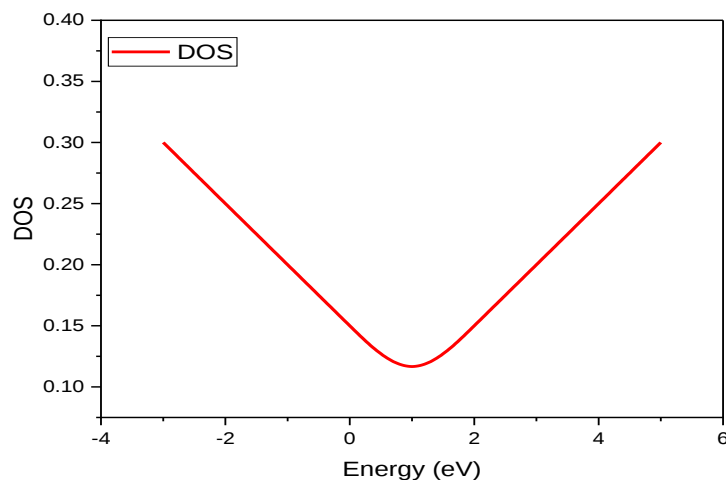


Figure 4: Density of States (DOS)

Figure. (4) presents the density of states (DOS) observed in the second thin film sample. The DOS profile, which is associated with energy levels, exhibits peaks and troughs that reflect the quantum landscape of the material. These arrangements provide insights into the fundamental electrical structure and introduce a novel approach to material investigation.

Sample 3: Electronic Band Structure

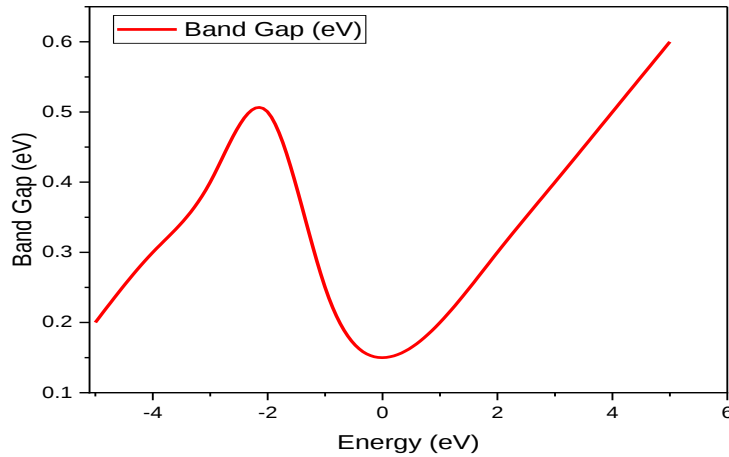


Figure 5: Electronic Band Structure

The electrical band structure of the third thin film is depicted in **Figure (5)**, which provides an enlarged view of the energy levels and the Brillouin zone. The band structure exhibits dynamic shifts that present potential for the customization of electrical properties. The visualization of electron movement within the bands offers valuable insights into the potential applications of the material.

Sample 3: Density of States (DOS)

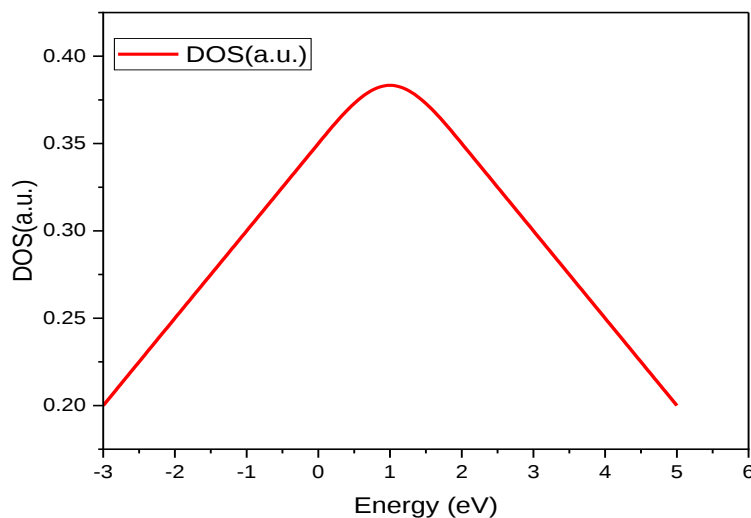


Figure 6: Density of States (DOS)

Figure (6) illustrates the density of states (DOS) within the third thin film specimen. The relationship between energy levels and density of states (DOS) is intricately connected, revealing the intricate structure of quantum energy states. The presence of peaks and valleys in a material's electronic landscape is indicative of its various electronic arrangements.

Firstly, the Comparison between Electronic Band Structures

The energy levels and Brillouin zones for three independent samples are depicted in **Figures (1), (3), and (5)**, which represent Electronic Band Structure plots. The first sample (**Figure (1)**) demonstrates the presence of an inherent band gap that regulates its electrical characteristics, whereas the second sample (**Figure (3)**) indicates dynamic changes in its band structure, suggesting the possibility of changing electrical properties. On the other hand, Sample 3 (**Figure (5)**) exhibits an amplified representation of its electronic band structure, thereby highlighting the possible prospects for customized electronic characteristics, which might be advantageous in several fields such as electronics or optics.

Secondly Comparison between the Density of States (DOS):

The Density of States (DOS) diagrams, as depicted in **Figures (2), (4), and (6)**, provide valuable insights into the quantum energy states present in the three examined samples. The DOS profile depicted in Sample 1 (**Figure (2)**) exhibits distinct peaks and valleys, offering a comprehensive depiction of its electrical structures. In the case of Sample 2 (**Figure (4)**), the density of states (DOS) profile exhibits peaks and troughs that correspond to its quantum landscape. However, it is expected that there would be some differences in these features compared to Sample 1. Sample 3 (**Figure (6)**) exhibits a discernible density of states (DOS) profile characterized by prominent peaks and valleys, indicating distinctive electronic configurations that deviate from those observed in Samples 1 and 2. The aforementioned comparisons highlight the discrepancies in electronic band structures and density of states (DOS) profiles observed in the three samples, thereby demonstrating the significant impact that modifications in film composition or structure can have on their electronic properties. These insights have immense value in customizing materials for specific purposes within disciplines such as electronics or optics.

4. Conclusions

In the passionate endeavor to comprehend the complexities of material behavior, we direct our attention toward the captivating domain of thin film simulations. The mutually beneficial relationship between VASP's computational capabilities and Origin's visualization expertise enhances our understanding of the intricate nature of thin film complexity. By utilizing these

communication pathways, we navigate the extensive realm of atomic and electronic interactions, acquiring valuable knowledge that spans from the minuscule to the grand scale. This process facilitates significant advancements in the field of materials science and technology, leading to transformational advances.

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