

# Note:Applying the Brillouin Zone and Band Gap Leveraging AB Initio Calculation for Digital Well-Being:In-Depth Analysis of Band Structures in Information Spaces Insights from Solid-State Physics

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**Abstract:** The efforts of this Note are aimed at understanding various phenomena in digital space that are incomplete and difficult to define, and to translate them into language from research fields that are based on existing large-scale experimental data. Information diffusion and user behavior patterns in digital space are often hard to intuitively capture, and the principles and mechanisms behind them are difficult to articulate. To address this challenge, we have drawn on first-principles methods in physics, particularly solid state physics. This approach is known to be effective in analyzing the behavior of real physical materials at the atomic level and in understanding the electronic properties and bonding structures of materials. We have attempted to apply physical concepts based on first-principles calculations, in particular concepts such as first Brillouin zones, band gaps, and reciprocal lattice vectors, to digital space as a metaphor. This theoretical framework allows us to quantitatively and logically infer the behavior and trends of incomplete and ambiguous digital data and phenomena. For example, the "first Brillouin zone" of information in digital media indicates the potential sphere of influence of that information, and the band gap defines the threshold of influence for the information to be widely accepted. In addition, the reciprocal lattice vector serves as a boundary that indicates the limits of information characteristics and is an indicator of the degree to which a particular piece of information resonates with users. With this theoretical supplement, our research goes beyond the mere analysis of phenomena in the digital space and provides new methods for understanding and predicting the behavior of imperfect data and uncertain digital media. This will hopefully enable digital media creators and platform designers to develop strategies for building healthier and more sustainable digital environments. This research will provide both the theoretical foundation and practical applications as part of an effort to define and verbalize the behavior of information in digital spaces.

**Keywords:** AB Initio Calculation, First Brillouin Zone, Band Gap Theory, Reciprocal Lattice Vectors, Information Dissemination, Quantum Mechanics in Digital Media, Theoretical Framework for Digital Health, Influence Threshold in Information Spread

## 1. Introduction

The use of first-principles(AB Initio Calculations) concepts and methods in applications from materials science to the field of digital media, particularly in the analysis of the diffuse structure of information and its influence in digital space, offers a new theoretical approach.

First-principles calculations(AB Initio Calculations) are a powerful method for understanding the electronic structure and physical properties of materials at the atomic level. The method directly calculates the behavior of atoms and electrons by solving the Schrödinger equation and its approximations. Below we add a theoretical supplement on the key points of

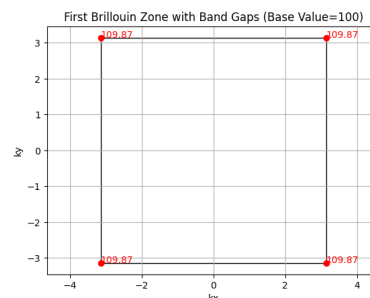


Fig. 1: First Brillouin Zone with Band Gaps



Fig. 2: First Brillouin Zone of a Square Lattice

first-principles calculations (AB Initio Calculations) and their application to materials science.

Total Energy and Structural Optimization, First-principles calculations (AB Initio Calculations) are based on the total energy in the calculation cell. The structure in which the total energy is minimized is considered the most stable structure of the material. The forces derived from the total energy can be used to optimize the positions of the atoms and identify the stable structure of the substance.

The energy band structure shows the distribution of possible energies for the electrons in a substance. From this structure, we can understand the electronic properties of a material, such as whether it is a metal, an insulator, or a semiconductor.

Lattice constants allow us to understand how a material responds and changes its lattice under pressure by comparing it to experimental values. The concept of the most stable structure predicts the most stable structure of a substance at absolute zero, which is useful for analyzing phase transitions and unusual physical properties. The concept of magnetism helps students understand the type of magnetism exhibited by a material (e.g., ferromagnetic, antiferromagnetic) and contributes to the design of magnetic materials. The concept of elastic constants predicts the mechanical properties of materials (e.g. Young's modulus) and verifies its accuracy through comparison with experimental values. Impurity formation energies and diffusion barriers calculate the behavior of impurities in a material and the energy barriers to diffusion. Surface and interface energies evaluate the strength of interactions through the energy possessed by the surfaces of materials and interfaces between dissimilar materials. Phonon dispersion analyzes lattice vibrations that affect the thermal and mechanical properties of materials. Band gap and density of states, which are essential for semiconductor properties and optoelectronic device design, are calculated.

These theoretical analyses provide a deep understanding of the fundamental properties of materials and can contribute to the design of new materials and improvement of the perfor-

mance of existing materials. The first-principles approach not only complements experimental studies in materials science, but also helps to understand unknown materials and complex phenomena. A powerful method for understanding the electronic state and local structure of matter, first-principles calculations reveal the band structure of matter using the relationship between the wavenumber  $k$  and the intrinsic energy  $\varepsilon_k$ . This dispersion relationship is essential to understanding the electronic properties of materials, and by plotting the relationship between energy and wavenumber, one can determine whether a material is a metal, insulator, or semiconductor.

Applying these physical concepts as metaphors to understand the structure of information dispersion and influence in digital media is an effective approach to verbalize and understand the various phenomena of digital space, which are imperfect and difficult to define. Specifically, by defining the "first Brillouin zone" of information in digital media and locating it as a "reciprocal lattice vector" of information properties, we can model the diffusion potential of information and the threshold of social acceptance. This makes it possible to infer and quantify the behavior and diffusion mechanisms for incomplete digital data and trends.

Furthermore, in conjunction with X-ray absorption spectroscopy, it provides a means to empirically test the correlation between theoretical predictions based on first-principles calculations and actual behavior. In the empirical analysis of information diffusion and influence in digital media, this approach provides an important indicator for understanding how specific information and topics are accepted and shared.

The integration of this theoretical framework and empirical approach is expected to lay a new foundation for better understanding information behavior and trends in the digital space and for developing effective information diffusion strategies. This can be an important step toward improving digital health and creating a more sustainable digital media environment.

Our goal is to understand and verbalize various phenomena in digital space that are imperfect and difficult to define. Information diffusion and user behavior patterns in digital space are often hard to intuitively capture, and the principles and mechanisms behind them are difficult to articulate. To address this challenge, we have drawn on first-principles methods in physics, particularly solid state physics. This approach is known to be effective in analyzing the behavior of real physical materials at the atomic level and in understanding the electronic properties and bonding structures of materials.

We have attempted to apply physical concepts based on first-principles calculations, in particular concepts such as first Brillouin zones, band gaps, and reciprocal lattice vectors, to digital space as a metaphor. This theoretical framework allows us to quantitatively and logically infer the behavior and

trends of incomplete and ambiguous digital data and phenomena. For example, the "first Brillouin zone" of information in digital media indicates the potential sphere of influence of that information, and the band gap defines the threshold of influence for the information to be widely accepted. In addition, the reciprocal lattice vector serves as a boundary that indicates the limits of information characteristics and is an indicator of the degree to which a particular piece of information resonates with users.

With this theoretical supplement, our research goes beyond the mere analysis of phenomena in the digital space and provides new methods for understanding and predicting the behavior of imperfect data and uncertain digital media. This will hopefully enable digital media creators and platform designers to develop strategies for building healthier and more sustainable digital environments. This research will provide both the theoretical foundation and practical applications as part of an effort to define and verbalize the behavior of information in digital spaces.

The goal of this notebook effort is to understand and verbalize various phenomena in digital space that are incomplete and difficult to define. Information diffusion and user behavior patterns in digital space are often hard to intuitively capture, and the principles and mechanisms behind them are difficult to articulate. To address this challenge, we have drawn on first-principles methods in physics, particularly solid state physics. This approach is known to be effective in analyzing the behavior of real physical materials at the atomic level and in understanding the electronic properties and bonding structures of materials.

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tions as part of an effort to define and verbalize the behavior of information in digital spaces. Applying the concepts of first-principles (AB Initio Calculations) computation to the information space of digital media may provide insight into unknown trends in the information space, including In terms of the analogy between total energy and structural optimization, "total energy" in digital media can represent the overall "activity" or "dynamism" within the information ecosystem. For example, it can be an indicator of how active a particular topic or discussion is and how that activity affects the ecosystem as a whole. In terms of optimizing the information ecosystem, minimizing this total energy may provide the most balanced and stable flow of information. This approach can help in developing strategies to curb the spread of information overload and misinformation on digital media and create a healthier information environment.

In the energy band structure metaphor, the energy band structure in digital media can be used as a metaphor for how information and ideas "flow" or what "path" they take. Certain information may reach the "conduction band" and spread widely, whereas some information may remain in the "valence band" and be shared only to a limited extent. We can also understand the ease of diffusion of information and barriers between communities through the concept of a "band gap," which indicates the ease of transfer of information between different communities.

In the magnetism analogy, the "magnetism" of information or ideas can indicate how well the information attracts people and is shared within a community. Information that is ferromagnetic has the potential to attract a large number of people and be spread quickly and widely. In contrast, information that is antiferromagnetic or weakly magnetic may attract limited interest and be shared only within a small area. Using this analogy can provide insight into understanding why certain information or topics are popular in some communities and receive little attention elsewhere.

Through these analogies, we will be able to understand the behavior of information and community dynamics on digital media and explore new information flows and diffusion mechanisms. These insights can also be used for a variety of applications, such as designing digital media, developing information strategies, and managing misinformation.

By applying the concepts of first-principles computation to the information space of digital media, we can explore the following unknown trends in the information space.

As an analogy to the lattice constant, the "lattice constant" in digital media can be used as a metaphor for the density or intensity of relationships among community members. By analyzing the community's response to pressure (external influences), we can understand how flexible the community is to any external change, or how susceptible the structure is to change due to pressure.

As a metaphor for the most stable structure, we can think of the structure in which information flows and communication patterns are most efficient and stable as the "most stable structure." We seek the optimal structure that will maintain a stable flow of information through the various "temperatures" (changes in environment and circumstances) that a community may face.

As an analogy to magnetism, the "magnetism" of information and ideas in digital media indicates the ability of that information to attract people and be shared within the community. Information that is ferromagnetic attracts more people and spreads quickly, whereas information that is antiferromagnetic may receive less attention. Through this concept, one can analyze why certain information becomes popular or is ignored.

As a metaphor for elastic constants, we can model the degree to which content and communities on digital media can withstand external "forces" (new information, trends, controversies, etc.) as "elastic constants." This analogy can be used to understand how flexible a community is and how it reacts to external influences.

Through the metaphor of "impurity formation energy" and "diffusion barriers," we can examine how new ideas and information are accepted or rejected within a community. High formation energy can indicate that new information is less acceptable to the community, while diffusion barriers can represent factors that prevent information from spreading within the community. As surface energy and interface energy, the strength of interactions between different communities and platforms can be analyzed through the metaphor of "surface energy" and "interface energy" to analyze the strength of ties between them and how information is exchanged.

As a metaphor for phonon dispersion, we can compare how information and trends propagate within a community. Using this analogy, it is possible to simulate the patterns in which information spreads and at which points it propagates most strongly.

By thinking of the "energy" required for a community to accept new information as a "band gap," thresholds of acceptability for different information and ideas for different information and ideas. A low bandgap indicates that information is easily accepted, while a high bandgap means that it is difficult to accept.

Through these analogies, we can gain a deeper understanding of information behavior and community dynamics in digital media and propose new approaches to explore new information flows and diffusion mechanisms. This will allow us to develop strategies to help manage information, curb misinformation, and maintain community health.

## 2. Discussion: "First Brillouin zone" in Digital Media

The application of first-principles calculations (Ab Initio Calculations) in materials science is transferred to the analysis of information diffusion structures and their influence in the field of digital media, providing a new theoretical framework for digital communication. This is based on first-principles calculations, a powerful tool used to analyze the electronic state and local structure of materials, and is inspired by the method of deriving the band structure from the relationship between the wavenumber  $k$  and the intrinsic energy  $\varepsilon_k$  exhibited by a material. This relationship, or dispersion relation, is essential to elucidating the electronic properties exhibited by materials and is obtained by plotting the relationship between energy and wavenumber to determine whether a material is a metal, insulator, or semiconductor.

Applying these physical concepts as metaphors to the analysis of information dispersion and influence in digital media can be an effective way to formulate and better understand the uncertain and complex phenomena of digital space. The definition of the "first Brillouin zone" in digital media and the localization of information characteristics as "reciprocal lattice vectors" can be used to model the diffusion potential and social acceptance thresholds of information, allowing us to infer and quantify the behavior and diffusion mechanisms of uncertain and fragmented digital data and trends. This enables us to infer and quantify the behavior and diffusion mechanisms of uncertain and fragmentary digital data and trends.

Furthermore, in conjunction with X-ray absorption spectroscopy, it provides a means to empirically verify correlations between theoretical predictions based on first-principles calculations (Ab Initio Calculations) and actual behavior. In the empirical analysis of information diffusion and influence in digital media, this approach provides an important indicator for elucidating how certain information and topics are accepted and shared.

This integration of theoretical frameworks and empirical approaches is expected to lay a new foundation for better understanding information behavior and trends in the digital space and for developing effective information diffusion strategies. This will be an important step in contributing to the promotion of digital health and the creation of a more sustainable digital media environment. This theoretical supplement will enable a deeper understanding of first-principles calculations in materials science and their application to digital media, and will provide a more accurate picture of information flows and their effects in an uncertain digital environment.

By applying the concepts of dispersion relations and band structure, which relate wave numbers to energy eigenvalues, to the information space of digital media, we may explore the following unknown trends in the information space.

In terms of dispersion relations and band structure of information space, "wavenumber" in digital media can symbolize the characteristics or "wave motion" of a particular piece of information or topic. The corresponding "energy eigenvalue" can represent the influence or diffusion capacity of that information. Using this analogy, it is possible to analyze how different topics and information diffuse and how much influence they have.

In terms of band gaps and information transferability, the "band gap" in a band structure can represent the "energy threshold" required for information to be transferred in digital media. In an information space with a large band gap, new information and ideas require greater influence and stimulation to gain widespread acceptance. This can be an indicator of whether a community is conservative or open to new information.

In terms of band dispersion and the bound state of information, if the dispersion of a band is weak, the electrons belonging to that band are considered more bound. In digital media, this can indicate that information is strongly anchored within a particular community or platform and is less likely to diffuse outside. Conversely, when dispersion is strong, information can spread more freely and have far-reaching effects.

System Stability and Information Ecosystem Health, By comparing the band structure of different systems, we can discuss which system is more stable. Similarly, by comparing different information ecosystems or communities on digital media, we can assess which has a healthier and more sustainable information flow.

Using these analogies can provide new perspectives to explore trends in unknown information spaces, such as the behavior of information on digital media, interactions between communities, and the receptivity of new information. These insights can also provide a basis for developing strategies to help manage information, curb misinformation, and maintain community health.

## 2.1 Bridging Physical and Digital Realms

The application of large-scale computational methods and chemical reaction simulations, as employed in condensed matter physics and materials science, to the vast information diffusion processes in digital spaces offers significant implications and opportunities. This discourse explores the potential of leveraging first-principles calculations, particularly those used in the investigation of honeycomb lattice structures and two-dimensional materials, to elucidate and predict complex phenomena in digital spaces that are yet to exhibit discernible patterns.

First-principles calculations (Ab Initio Calculations), grounded in fundamental laws of physics, provide a robust framework for understanding material properties at an atomic level. The adaptation of these methodologies to digital infor-

mation spaces could establish a new paradigm where information flow and its intricacies are mapped onto physical models, such as the honeycomb lattice, renowned for its unique properties in materials like graphene.

## 2.2 Honeycomb Lattice as a Model for Digital Phenomena

The honeycomb lattice structure, with its high degree of symmetry and distinct electronic properties, offers an intriguing analogy for the complex networks within digital spaces. Just as electrons move and interact within this lattice, leading to phenomena like the emergence of Dirac fermions, information packets in a digital space could be conceptualized similarly, with their spread and interaction patterns shedding light on underlying digital dynamics.

## 2.3 Advantages of First-Principles Approaches

**Predictive Power:** First-principles calculations can predict material behavior under various conditions without empirical input. Applied to digital spaces, this approach could forecast information spread under different network conditions, identifying potential viral patterns or bottlenecks.

**Understanding Complex Interactions:** Just as these calculations reveal complex electron interactions leading to material properties, they could unravel the multifaceted interactions between digital entities, enhancing our understanding of digital ecosystems.

**Designing Optimal Pathways:** In materials science, these calculations aid in designing materials with desired properties. Similarly, they could help design optimal information dissemination strategies in digital spaces, maximizing reach and engagement while minimizing misinformation.

## 2.4 Challenges and Considerations

While the analogy between physical and digital spaces is compelling, several challenges and considerations need addressing:

**Complexity of Digital Spaces:** Unlike physical systems, digital spaces are influenced by human behavior, cultural nuances, and non-linear dynamics, adding layers of complexity to the modeling process.

**Adaptation of Physical Models:** Translating physical models to represent digital phenomena necessitates novel theoretical frameworks and computational algorithms that can capture the essence of information flow in digital spaces.

**Ethical and Privacy Concerns:** The application of such models to analyze and influence digital spaces must be

navigated with a keen awareness of ethical considerations and privacy implications.

In conclusion, while the application of first-principles calculations (AB Initio Calculations) to digital information spaces presents a promising frontier, it requires interdisciplinary collaboration, innovative modeling approaches, and a careful consideration of ethical implications to fully realize its potential.

### 3. Bridging Physical and Digital Realms<sup>2</sup>

#### 3.1 First Brillouin Zone

The First Brillouin Zone is the Wigner-Seitz cell in the reciprocal lattice space of a crystal, reflecting the fundamental periodicity of the crystal. Each point within this zone corresponds to a wave vector  $\mathbf{k}$ , influencing the phase factor of the electron's wave function. Crossing the boundary of the First Brillouin Zone, the electron wave function is replicated at another point within the same zone, fully describing the fundamental physical properties within this zone.

#### 3.2 Band Gap

The band gap is the energy difference between the valence band and the conduction band, serving as a crucial indicator to distinguish whether a material is a metal, an insulator, or a semiconductor. The magnitude of the band gap determines the material's ability to absorb energy (e.g., light) from external sources, facilitating electron transitions to the conduction band. The band gap  $E_g$  is expressed by the following equation:

$$E_g = E_c - E_v$$

Here,  $E_c$  represents the minimum energy of the conduction band, and  $E_v$  represents the maximum energy of the valence band.

#### 3.3 Tight-Binding Model

The Tight-Binding Model is one of the quantum mechanical models used to describe the electronic states of atoms or molecules. In this model, conduction is understood as electrons "jumping" between neighboring atoms. By linearly combining wave functions based on the electronic states of atoms, the electronic wave function of the entire crystal is constructed, determining the energy  $E$  as a function of the wave vector  $\mathbf{k}$  as follows:

$$E(\mathbf{k}) = E_0 + \sum_{\Delta} t_{\Delta} e^{i\mathbf{k} \cdot \Delta}$$

Here,  $E_0$  represents the on-site energy of the atomic electronic state,  $t_{\Delta}$  represents the hopping energy between neighboring atoms, and  $\Delta$  represents the vector between neighboring atoms.

Through these equations and computational processes, utilizing the concepts of the First Brillouin Zone, Band Gap, and Tight-Binding Model, one can gain a deeper understanding of the mechanisms of information diffusion and aggregation, elucidating the physical principles behind undefined patterns and unpredictability in the flow of information in digital spaces.

#### 3.4 Band Structure of Information in Digital Media

When exploring the concept of "band structure of information" in digital media, inspiration can be drawn from the theory of band structure in materials. The band structure in materials is typically defined based on Bloch's theorem, represented by the eigenvalues of electron energy  $E(k)$ , dependent on wave vector  $k$ . This relationship is expressed by the following equation:

$$E(k) = \frac{\hbar^2 k^2}{2m} + U(k)$$

Here,  $\hbar$  is the reduced Planck constant,  $m$  is the mass of the electron, and  $U(k)$  is the periodic potential, a function of wave vector  $k$ .

To apply this concept to the context of digital media, one can analogize the "characteristics" of information or content to the wave vector  $k$ , and its "influence" or "diffusion ability" to the energy  $E$ . The "characteristics" of information can be defined based on various elements such as uniqueness, complexity, or relevance of the topic. On the other hand, "influence" can be measured by how widely the information is accepted and shared.

#### 3.5 Band Structure Model of Information in Digital Media

To model the band structure of information in digital media, a simplified relationship can be considered as follows:

$$I(k) = a \cdot k^2 + b$$

Here,  $I(k)$  represents the influence of a specific information characteristic  $k$ , and  $a$  and  $b$  are appropriate constants adjusting the ease of diffusion of information and the level of basic influence. In this model, it demonstrates that as the characteristics of information increase, its influence increases quadratically.

#### 3.6 Applications and Prospects

By using this model, the "band structures" of different topics or contents in digital media can be theoretically analyzed,

predicting their ease of diffusion and acceptability within communities. For instance, by altering the value of  $a$ , one can adjust the ease of change in influence regarding specific information characteristics, understanding which information characteristics diffuse most effectively.

Furthermore, by introducing the concept of a band gap, one can consider the "minimum influence" necessary for certain information to be accepted within a community. This allows evaluating how innovative or influential information needs to be and analyzing the health and openness of its information ecosystem.

This theoretical framework would also serve as a foundation for devising strategies to enhance the health and sustainability of digital media.

### 3.7 First Brillouin Zone

The First Brillouin Zone is a concept associated with crystal lattices, playing a crucial role in solid-state physics and first-principles calculations. It refers to the most significant region in the reciprocal space (or  $k$ -space) of a crystal lattice. Also known as the Wigner-Seitz cell in the reciprocal lattice, it is a region enclosed by planes positioned halfway between the reciprocal lattice points, centered around the origin.

### 3.8 Definition of the First Brillouin Zone

In crystals, atoms or molecules are arranged in periodic patterns, described by lattices in real space. Each lattice point is specified by lattice vectors  $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$  ( $n_1, n_2, n_3$  are integers,  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are primitive lattice vectors). Reciprocal space corresponds to the space associated with this real-space lattice and is composed of reciprocal lattice vectors  $\mathbf{G} = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3$  ( $m_1, m_2, m_3$  are integers,  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are primitive reciprocal lattice vectors).

The First Brillouin Zone is delimited by half the distance from the origin to the nearest reciprocal lattice point and is essential for understanding fundamental properties of wave functions such as electronic states and phonon states.

### 3.9 Importance of the First Brillouin Zone

The eigenvalues of electrons at any point within the First Brillouin Zone, denoted by  $E(\mathbf{k})$ , determine the electronic band structure of a crystal. According to Bloch's theorem, electron wave functions within a crystal can be described using wave vectors  $\mathbf{k}$  within the First Brillouin Zone, thereby determining the electronic properties of the crystal.

First-principles calculations, particularly methods like density functional theory (DFT), compute the ground state energies and other physical properties of materials by integrating within the First Brillouin Zone. This process involves a technique called  $k$ -point sampling, where representative points ( $k$ -points) within the First Brillouin Zone are selected

to calculate the eigenvalues at those points and derive the properties of the material.

The First Brillouin Zone is a central concept in understanding the behavior of quantum particles such as electrons and phonons within crystals, providing the foundation for calculating the electronic properties and many other physical properties of materials in first-principles calculations. This understanding directly contributes to the design of new materials, improvement of existing material properties, and even the discovery of new phenomena in materials science.

## 3.10 Applying the Concept of the First Brillouin Zone to Digital Media

To apply the concept of the First Brillouin Zone to the information space of digital media, it is necessary to understand the characteristics of information and the structure of its diffusion.

### 3.11 What is the First Brillouin Zone?

In the reciprocal lattice space of a crystal lattice, the First Brillouin Zone is the initial region enclosed by planes positioned halfway between the reciprocal lattice points, centered around the reciprocal lattice points. This serves as the fundamental cell in reciprocal space representing the basic periodicity of the crystal. Mathematically, the First Brillouin Zone is defined by reciprocal lattice vectors  $\mathbf{G}$  and is expressed as:

$$\mathbf{G} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

Here,  $h, k, l$  are integers, and  $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$  are primitive reciprocal lattice vectors.

To apply the concept of the First Brillouin Zone to the information space of digital media, we consider the characteristics of information (such as topic complexity or uniqueness) as analogs of reciprocal lattice vectors. We understand the "wave number"  $k$  of information as its position in the "reciprocal space" of information characteristics. We can model the diffusion ability and influence of information as eigenvalues  $E$ , considering  $E(k)$  as a function of information characteristics  $k$ .

To define the band structure of information, we need to define an appropriate function  $E(k)$ . For example, linear or quadratic functions can be considered as simple models:

$$E(k) = a + bk$$

$$E(k) = a + bk^2$$

Here,  $a$  represents the basic level of influence, and  $b$  represents the rate of change of influence with respect to information characteristics.

By using this theoretical framework, we can understand how different information characteristics diffuse and are accepted. For instance, defining the "First Brillouin Zone" of

information on a specific platform in digital media allows analyzing how information behaves within it. Analyzing the band gap of information allows evaluating the "stimulus threshold" required for new ideas or topics to be widely accepted.

## 4. Tight-Binding Model in First Principles Calculations

The Tight-Binding Model (TBM) in first principles calculations is one of the essential methods for understanding the electronic properties of materials. This model is widely used, especially in solid-state physics, for computing electronic band structures. In the Tight-Binding Model, the energy associated with electrons hopping between atoms is considered, describing the electronic state of the entire crystal.

The starting point of the Tight-Binding Model is to consider the wave functions of electrons localized on each atom in the crystal (atomic orbitals). It is assumed that any electronic state in the crystal can be approximated by a linear combination of these atomic orbitals (Linear Combination of Atomic Orbitals, LCAO). That is, the electronic wave function  $\Psi(\mathbf{r})$  in the crystal is expressed as a linear combination of individual atomic orbitals  $\phi_i(\mathbf{r})$ :

$$\Psi(\mathbf{r}) = \sum_i c_i \phi_i(\mathbf{r})$$

Here,  $c_i$  are coefficients of the linear combination, and  $\phi_i(\mathbf{r})$  represents the atomic orbital of the  $i$ th atom at position vector  $\mathbf{r}$ .

### 4.1 Hamiltonian and Energy Eigenvalues

The energy of electrons in the Tight-Binding Model is calculated using the Hamiltonian operator  $\hat{H}$ . The Hamiltonian includes both the on-site energy (electron energy within the same atom) and hopping energy (energy of electrons moving between different atoms).

$$\hat{H} = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_{i \neq j} t_{ij} |i\rangle\langle j|$$

Here,  $\varepsilon_i$  is the on-site energy of the  $i$ th atom,  $t_{ij}$  represents the hopping energy from the  $i$ th atom to the  $j$ th atom, and  $|i\rangle$  denotes the state of the  $i$ th atom in Dirac notation.

In first principles calculations (Ab Initio Calculations), the Tight-Binding Model is further refined to reflect the actual atomic interactions. Methods such as Density Functional Theory (DFT) are used, and calculations are based on the actual atomic potentials and electron densities. In DFT, the exchange-correlation potential is approximated, and the Schrödinger equation is solved, taking into account the interactions between electrons.

$$\hat{H}\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$

Here,  $\hat{H}$  is the Hamiltonian based on DFT, and  $E$  is the energy eigenvalue of the electron.

The Tight-Binding Model provides a powerful framework for understanding the electronic states in crystals. In first principles calculations, this model serves as a starting point for accurately computing the electronic properties of real materials. Particularly when combined with Density Functional Theory, it becomes possible to predict many physical properties such as electronic band structures, density of states, and optical properties of materials. These computational results are expected to directly contribute to the design of new materials and the improvement of properties of existing materials.

Applying the tight-binding model from first-principles calculations in the realm of digital media offers a novel approach to understanding how information and content are disseminated and consumed. In this application, information and content can be likened to electrons, while digital media platforms and networks can be analogized to crystal lattices.

To apply the tight-binding model in the context of digital media, it is necessary to first define the "atomic orbitals" of information and content. These represent the inherent characteristics or attributes of specific content (e.g., topic, style, target audience) and form the basic "energy states" of the content.

The tight-binding model for information in digital media might be represented as follows:

$$I(\mathbf{c}) = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_{i \neq j} t_{ij} |i\rangle\langle j|$$

Here,  $I(\mathbf{c})$  represents the "influence" or "spread" of information at a specific content characteristic vector  $\mathbf{c}$ ,  $\varepsilon_i$  denotes the inherent "influence" of content  $i$ , and  $t_{ij}$  signifies the "spread" from content  $i$  to content  $j$ . The notation  $|i\rangle$  symbolizes the state of content  $i$  in an abstract representation.

Utilizing this model allows for the quantitative analysis of how specific content or information diffuses and interacts within digital media platforms. For instance, if the "hopping energy"  $t_{ij}$  between contents related to a certain topic is high, it can be anticipated that the topic will easily spread within the platform, possessing significant influence.

Moreover, this model could assist content creators and marketers in devising strategies to optimize the spread and influence of specific content by adjusting its characteristics. It could also provide insights into how digital media platforms should be designed and what types of content are likely to succeed on the platform.

The application of the tight-binding model in the information space of digital media offers a new methodology for understanding and optimizing the dissemination mechanisms of information and content. This approach could contribute to building a theoretical framework to assist in strategizing for enhancing information spread and aiding decision-making in the design of digital media platforms.

## 4.2 Determining Information Characteristics $k$ for Each Pattern in the First Brillouin Zone

To determine the pattern-specific information characteristics  $k$  in the first Brillouin zone, an approach using reciprocal lattice vectors is necessary. In a crystal lattice, the first Brillouin zone is defined as the first Wigner-Seitz cell in reciprocal lattice space. This cell is the region surrounded by the closest reciprocal lattice points from the origin of the reciprocal lattice.

Reciprocal lattice vectors are determined by the primitive lattice vectors of the crystal lattice. For 2D and 3D lattices, the reciprocal lattice vectors  $\mathbf{b}_i$  are calculated as follows:

For 2D:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \hat{z}}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \hat{z})}$$

$$\mathbf{b}_2 = 2\pi \frac{\hat{z} \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \hat{z})}$$

For 3D:

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

Here,  $\mathbf{a}_i$  are the primitive lattice vectors of the real lattice, and  $\hat{z}$  is the unit vector along the z-axis.

Any point  $k$  within the first Brillouin zone is expressed as a linear combination of these reciprocal lattice vectors. That is,

$$\mathbf{k} = h\mathbf{b}_1 + k\mathbf{b}_2 (+/\mathbf{b}_3)$$

Here,  $h, k, (l)$  are integers representing coordinates in reciprocal lattice space. By varying these parameters, different points within the first Brillouin zone can be identified.

In the context of application to digital media, the concept of reciprocal lattice is abstracted into the space of information characteristics  $k$ , defining the "positions" of different information characteristics. To simulate this concept in Python, reciprocal lattice vectors need to be defined, and points within the first Brillouin zone need to be computed. However, it's important to note that the information characteristic space in digital media differs from physical crystal lattices, so conceptual adaptation is required when using this analogy.

Fig.3 shows to be a graph with the title "Energy Band Structure Analogy for Digital Media Information Flow". It uses an analogy from physics, specifically semiconductor physics, to describe the spread of ideas in digital media.

This x-axis is labeled 'Idea Index' and spans from 0 to just over 50. It likely represents a sequence or a collection of ideas.

This y-axis is labeled 'Energy State' and extends from 1.0 to a bit over 2.0. In semiconductor physics, energy states refer to the energy levels that electrons can occupy. In this

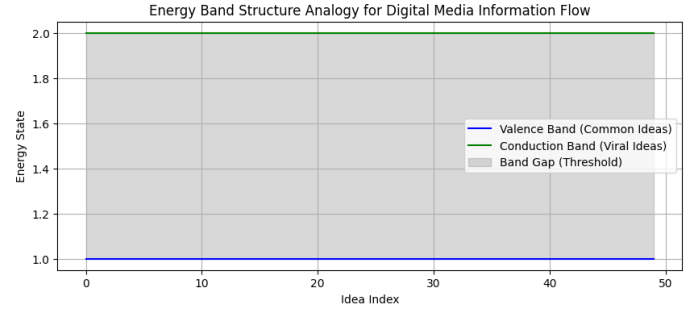


Fig. 3: Energy Band Structure Analogy for Digital Media Information Flow

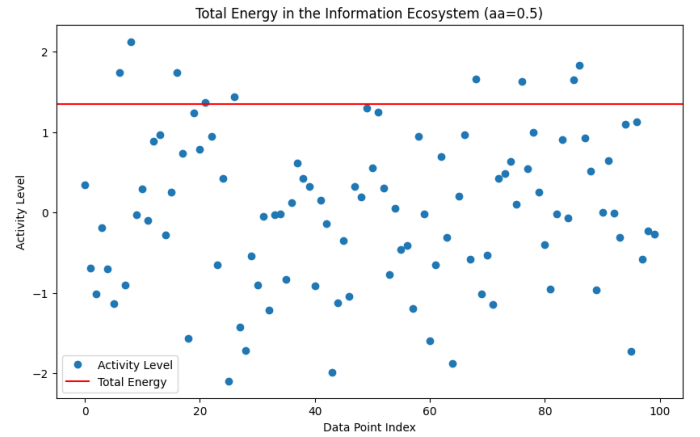


Fig. 4: Total Energy in the Information Ecosystem

analogy, it might refer to the "energy" or potential impact of an idea.

Valence Band (Common Ideas), This band is colored blue and is located at the bottom of the graph, suggesting it represents common, everyday ideas. Conduction Band (Viral Ideas), This green band is at the top, possibly representing ideas that have "gained energy" and become viral or widely circulated. There's a gap between the two bands, indicative of the threshold that ideas must cross to transition from being common to viral. This is akin to the energy gap electrons must overcome to move from the valence band to the conduction band in semiconductors.

But, there are no actual data points or lines within the bands, which suggests that the graph is a conceptual representation rather than an empirical one.

In summary, the graph uses the energy band diagram from semiconductor physics as a metaphor for how ideas might circulate in the digital media space. Common ideas exist in the lower energy valence band, while ideas that become viral are in the higher energy conduction band. The band gap represents the threshold that ideas must surpass to go from common to viral. The analogy can be used to understand the dynamics of information flow on social media and other digital platforms.

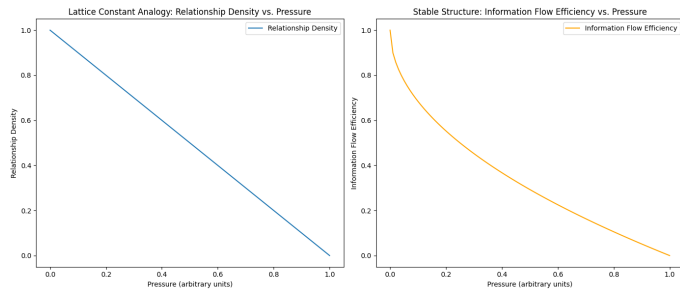


Fig. 5: 'Lattice Constant Analogy: Relationship Density vs. Pressure, Stable Structure: Information Flow Efficiency vs. Pressure

Fig.4 is titled "Total Energy in the Information Ecosystem (aa=0.5)" and it appears to represent a dataset related to activity levels in some kind of information ecosystem.

The x-axis is labeled 'Data Point Index' and extends from 0 to 100. It seems to correspond to individual measurements or events within the dataset. The y-axis is labeled 'Activity Level' and ranges from approximately -2 to 2. This axis likely measures the intensity or frequency of activity within the information ecosystem.

The blue dots scattered across the graph represent the activity level at various points. These are unevenly distributed, with no clear pattern, indicating that the activity level varies significantly across different data points.

There is a horizontal red line at the y-axis value of 1, labeled 'Total Energy'. This line could represent an average, threshold, or reference value for the total energy in the system.

The notation in the title "(aa=0.5)" could indicate a parameter or variable that's set to 0.5 for the current dataset. This parameter might control some aspect of the model or system being represented.

From the visual data, one can infer that: The activity levels vary widely, suggesting a dynamic or volatile information ecosystem. The total energy level is set at 1, which could imply that activity levels above this line are more intense or higher than average, while those below are less intense or lower than average. The parameter "aa" is likely a part of the model's settings or formula and its impact on the data is not directly clear from the graph alone.

Without additional context or data, it is difficult to draw more specific conclusions. However, the graph does provide a visual representation of the variation in activity levels within an information ecosystem, potentially useful for analyzing the distribution and intensity of activities.

Fig.5 shows two line graphs, each depicting a different relationship with respect to pressure in arbitrary units.

Lattice Constant Analogy: Relationship Density vs. Pressure\*\* The x-axis represents 'Pressure' in arbitrary units, ranging from 0 to 1. The y-axis represents 'Relationship Density', also ranging from 0 to 1. The graph features a

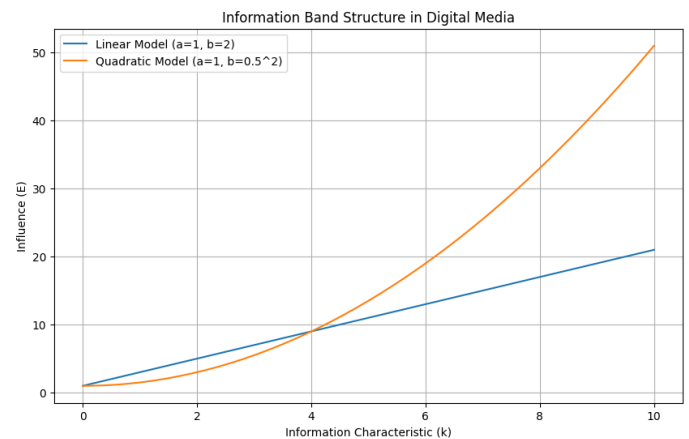


Fig. 6: Information Band Structure in Digital Media

single blue line that descends linearly from the top left to the bottom right, indicating that as pressure increases, the relationship density decreases. The 'Lattice Constant Analogy' in the title suggests a comparison to solid-state physics, where the lattice constant changes with pressure. Here, it's used metaphorically to describe how relationships within a system become less dense as external pressures increase.

Stable Structure: Information Flow Efficiency vs. Pressure, The x-axis is the same as in the left graph, showing 'Pressure' in arbitrary units. The y-axis now represents 'Information Flow Efficiency', which also spans from 0 to 1. This graph has an orange line that starts high on the y-axis and curves down steeply as pressure increases, which suggests that information flow efficiency decreases nonlinearly as pressure increases. The 'Stable Structure' in the title implies that this graph could be modeling the stability of an information system under pressure. As pressure goes up, the efficiency of information flow goes down, perhaps indicating that too much pressure can destabilize the system and lead to inefficiencies.

Overall, these graphs suggest that in the context of the analogy being used, both relationship density and information flow efficiency decrease as pressure increases. The linear decrease in relationship density could suggest a direct proportionality with pressure, while the nonlinear decrease in information flow efficiency might indicate that as pressure mounts, there's a more pronounced, perhaps exponential, drop in efficiency. The use of 'arbitrary units' for pressure implies a conceptual model rather than one based on empirical data.

Fig.6 is a line graph titled "Information Band Structure in Digital Media," showing two models that relate 'Influence' to 'Information Characteristic (k)'.

The equation for this model is given as 'a=1, b=2', suggesting a linear relationship where the slope is determined by 'b'. Since there's no explicit equation, we can assume it follows the form 'E = a + bk', where 'E' is influence and 'k' is the

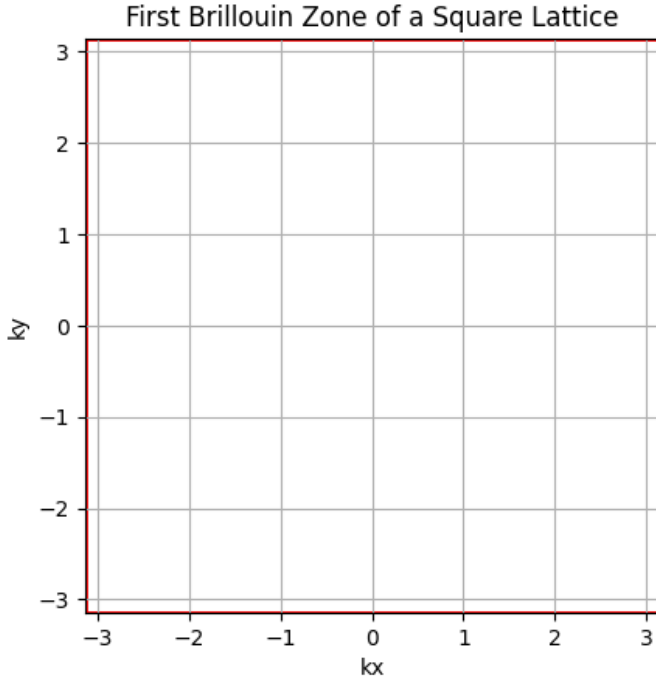


Fig. 7: First Brillouin Zone of a Square Lattice

information characteristic. As 'k' increases, the 'Influence' increases linearly, which is visualized by a straight line with a consistent slope. At 'k' equals 10, the 'Influence' is just above 20, which is consistent with the slope 'b=2' (starting from zero influence).

This model is described by the parameters 'a=1, b=0.5\*\*2', which implies a quadratic relationship, possibly of the form 'E = a + b\*\*k2'. Here, as 'k' increases, the 'Influence' increases at a growing rate, indicative of the squared relationship. The curve steepens as 'k' gets larger. At 'k' equals 10, the 'Influence' appears to reach 50, consistent with the quadratic nature where the influence grows much faster than the linear model.

Both lines start from the same point, suggesting that when 'k' equals 0, the 'Influence' starts at 'a', which is 1 for both models. The graph illustrates how different models of information influence can vary greatly with changes in the information characteristic 'k'. In digital media, this could represent how certain types of information or messages may have a much more significant influence as they grow in certain characteristics (like reach, engagement, or virality), especially as modeled by the quadratic equation, compared to a linear growth in influence.

Fig.7 shows a simple diagram labeled "First Brillouin Zone of a Square Lattice." The diagram has two axes:

This axis ranges from -3 to 3 and represents the crystal momentum in the x-direction within the reciprocal space of a crystal lattice.

Similarly, this axis ranges from -3 to 3 and represents

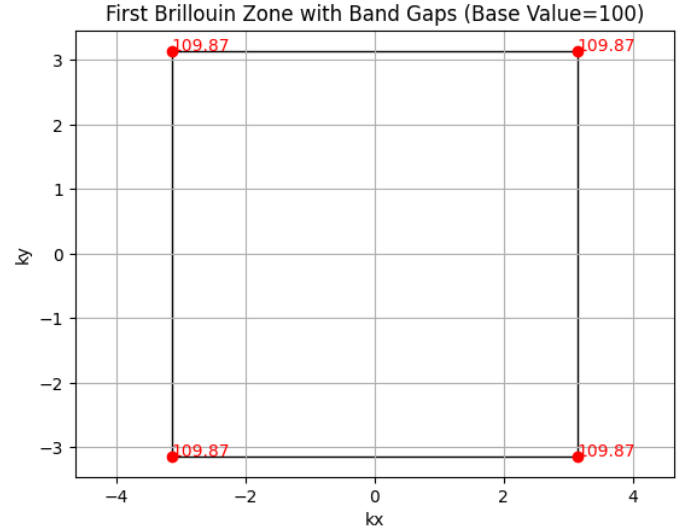


Fig. 8: First Brillouin Zone with Band Gaps

the crystal momentum in the y-direction within the reciprocal space.

The red square represents the boundaries of the first Brillouin zone for a square lattice. The Brillouin zone is a fundamental concept in the field of solid-state physics and crystallography. It describes the fundamental part of reciprocal space that contains unique information about the wave vectors that characterize the wave-like behavior of particles within the lattice.

The square shape of the Brillouin zone indicates that the real space lattice is also square because the first Brillouin zone is always the same shape as the real space lattice, though rotated and scaled in reciprocal space. The symmetry of the Brillouin zone about both the  $k_x$  and  $k_y$  axes indicates that the lattice has fourfold rotational symmetry in real space. The size of the first Brillouin zone is determined by the reciprocal lattice vectors, which are related to the spacing between atoms or unit cells in the real lattice.

In terms of physics, the boundaries of the Brillouin zone are significant because they are where the electron energy band structure can show effects such as band gaps, where no electron states can exist. This can lead to phenomena like the electronic band structure of solids, which is central to understanding the electrical, optical, and thermal properties of materials.

Fig.8 shows a diagram titled "First Brillouin Zone with Band Gaps (Base Value=100)" and features a graphical representation similar to a reciprocal lattice diagram from solid-state physics. As in the previous image, there are two axes labeled  $k_x$  and  $k_y$ , both ranging from -4 to 4, defining the reciprocal space.

The square outline remains the same, suggesting the diagram is showing the first Brillouin Zone for a square lattice.

Band Gaps, There are points marked in red at the corners of the Brillouin zone, with a value of "109.87" close to each point. These likely indicate the energy values at the edges of the Brillouin zone where band gaps occur. Band gaps are energy ranges in solid-state physics where no electron states can exist.

The title mentions a "Base Value=100," which might refer to the reference energy level from which the band gaps are measured. The band gaps are thus shown to have an energy level of "109.87" above this base value.

The diagram suggests that at the edges of the first Brillouin Zone, the energy levels are higher than the base value by "9.87." In the context of solid-state physics, these points might be significant for the electronic properties of the material because they indicate where the energy bands begin to separate, creating band gaps. This can affect how electrons move through the material, influencing its electrical and optical properties. The representation does not indicate how these band gaps might change within the Brillouin zone or how they relate to the rest of the band structure.

## 5. Perspect

The vision of this research is to apply ab initio computation and its concepts in physics to digital media analysis in order to gain a deeper understanding of the information distribution mechanisms in digital space and to propose strategies to promote digital health from a new perspective. Specifically, further research is expected to focus on the following points.

More precise mapping of information characteristics, further developing the concept of the "first Brunn zone" in digital space. This will include multiple dimensions of information, such as novelty, urgency, and relevance, and a quantitative analysis of how they affect the diffusivity and acceptability of information. Applying the concept of reciprocal lattice vectors in physics, we will develop new data analysis methods to analyze information distribution patterns on digital media. By combining machine learning and artificial intelligence techniques, we will construct algorithms to predict information diffusion trends and develop optimal content distribution strategies. Using the information bandgap concept, we will analyze the degree to which users are receptive to new information and ideas. Based on this analysis, we will propose content and interaction design guidelines that improve the user experience and encourage higher engagement. Utilizing a theoretical framework based on first-principles calculations, we will develop strategies to mitigate potential risks posed by digital media, such as information overload and fake news. We aim to contribute to the digital health of users by maintaining the health of digital communities and improving the quality of information. We will apply the theoretical models and analytical methods developed in this study to digital communication strategies in various fields, including educa-

tion, politics, and business. This will improve the efficiency of information transfer in various fields and contribute to the creation of a healthier and more productive digital environment.

Thus, applying the concepts of first-principles(AB Initio Calculations) computation to the analysis of digital media provides a new understanding of the mechanisms of information diffusion and a variety of approaches to promote the healthy distribution of information and user health in the digital space.

One of the benefits of this initiative is the application of the advanced theory of first-principles calculations(AB Initio Calculations) in physics to the analysis of digital media, providing a new perspective for understanding the mechanisms of information diffusion. This will enable a deeper understanding of the subtle behaviors and trends of information that cannot be captured by conventional analytical methods. Quantitative models based on physics can be used to mathematically analyze the characteristics of information and its social acceptance in digital media. This enables quantitative prediction and analysis of information diffusion patterns and influence thresholds in the digital space. By using the information bandgap concept to analyze the extent to which users are receptive to new information and ideas, it is possible to design content and interactions that contribute to an improved user experience. By mitigating the risks posed by digital media, such as information overload and fake news, and by suggesting strategies to maintain the health of digital communities, it is expected to improve the digital health of users. We provide theoretical models and analytical methods to improve the efficiency of information transfer in various fields such as education, politics, and business, thereby contributing to a healthier and more productive digital environment. As for the gap between theory and reality, a gap may exist between theory and the actual behavior of digital space when applying physics theory directly to the analysis of digital media. The complexity of digital space and the diversity of human behavior may not be fully captured. Physics concepts such as ab initio calculations and reciprocal lattice vectors are sophisticated and can be difficult for digital media professionals and practitioners to understand and implement. When modeling complex digital space phenomena with physics concepts, important elements and nuances may be lost, resulting in an overly simplified analysis. Analysis using advanced theoretical models requires large amounts of high-quality data, which are not always available. In addition, data biases and incompleteness may affect the results of the analysis. In addition, the dissemination of information and analysis of user behavior in digital media may raise ethical concerns in terms of privacy and personal data protection. Appropriate guidelines based on transparency and user consent must be established.

We propose a method of applying the concepts of first-

principles computation to the analysis of information diffusion and influence in digital media.

Inspired by the study of topological insulators in first-principles calculations (AB Initio Calculations), we can analyze the topology of information properties in digital media. By viewing information properties as topological features and investigating the behavior of information at the "boundaries" between different information properties, new phenomena in information diffusion and influence can be discovered. The concept of quantum entanglement is applied to analyze the relationships and interactions between information in digital media. By examining how different information properties "entangle" and influence each other, it is possible to understand and predict the collective diffusion patterns of information. Quantum dynamics methods, which describe the time evolution of electronic states of matter, will be applied to modeling the temporal diffusion process of information in digital media. This allows us to simulate the dynamic behavior of how specific information properties diffuse and increase or decrease in influence over time. Similar to the energy landscape of matter, the information properties of digital media are viewed as energy levels and their landscapes are analyzed. Using the principle of "energy minimization" of information properties, we predict the diffusion patterns and stable states of influence that information naturally favors.

These proposed analytical methods are expected to contribute to a better theoretical understanding of information diffusion in digital media and to the formulation of more precise and effective information diffusion strategies. These approaches will also lead to a better understanding of the health of digital media and the digital health of users.

Inspired by the application of first-principles calculations in materials science, its application to digital media analysis provides an innovative theoretical framework for understanding the structure of information dispersion and its influence. This includes the concept of dispersion relations based on the relationship between the wavenumber  $k$  and the eigenenergy  $\varepsilon_k$  used in the analysis of electronic states and local structures of matter. By applying this concept to the mechanism of information dispersion in digital media, we propose the following theoretical supplement and new analytical methods.

The concept of phonons (quantum of lattice vibration) in solid state physics is applied to digital media analysis to model the interaction between information properties. Using the phonon model, we theoretically analyze how information "vibration" and "resonance" affect information diffusion and clarify the dynamic relationships among information properties.

Inspired by the study of topological insulators in first-principles calculations, we introduce topological invariants into the band structure of information properties of digital media. This approach allows us to understand how informa-

tion diffusion and influence change when the band structure of information has topological properties, and to predict non-intuitive diffusion patterns and stability. Quantum walk is a fundamental concept in quantum information processing that describes the propagation of particles in terms of quantum dynamics. Quantum walk models of information in digital media can be built to unravel the complex patterns of how information diffuses through digital networks. This allows us to analyze in detail the impact of specific network structures and user behavior on information diffusion.

Quantify the correlation between different information sources and content in digital media by applying the concept of quantum entanglement. The measurement of information entanglement reveals the interdependencies between information and their strength, and provides a new metric for evaluating the influence and credibility of information.

These theoretical supplements and new analytical methods provide powerful tools for better understanding the behavior of information and its diffusion dynamics in digital media. Furthermore, these approaches are expected to provide important insights in developing strategies to improve information quality, foster user engagement, and enhance digital health.

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