

# First-Principles Calculations for Tuning Digital Information Propagation by Applying N-type and P-type Doping Mechanisms in Graphene

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**Abstract:** In this note, we propose to analyze the effects of nand p-type doping on graphene using first-principles calculations and apply the results to social simulations of the diffusion mechanisms of fake news in digital communication. The electronic properties of graphene and its tunable conductivity due to doping provide a useful metaphor for modeling changes in information flow and receptivity. n-type doping accelerates the propagation of information and p-type doping inhibits its spread, using the analogy that the propagation of fake news is a function of the doping type. dynamics from a new perspective. This research will examine a new theoretical framework approach to counter fake news by integrating physics and social science.

**Keywords:** First Principles Calculation, Social Simulation, Graphene, N-type Doping, P-type Doping, Fake News Diffusion, Information Propagation, Digital Communication, Conductivity Modulation, Fusion of Physics and Social Sciences

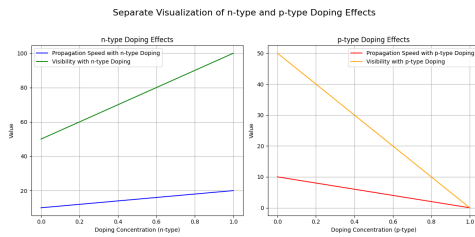


Fig. 1: Network Belief States susceptibility

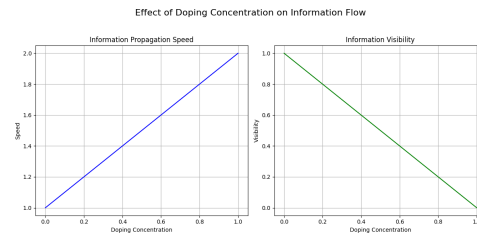


Fig. 2: Actual Reach, Speed, Spread

## 1. Introduction

First-principles calculations are methods for predicting the properties and behavior of matter based on physical laws and are used primarily in the fields of physics and chemistry. Starting from fundamental building blocks such as atoms and electrons, these calculations are powerful tools for understanding the properties of complex material systems. At the core of this approach is the ability to verify consistency between experimental results and unknown phenomena through predictions based on fundamental principles.

Applying this process of computational experimentation and verification to social simulation means opening new avenues for deepening the relationship between theory and reality in the social sciences. Social simulation aims to model and understand individual behavior, social interactions, and the resulting collective phenomena. By incorporating a first-

principles computational approach, it is possible to gain a more principled view of the fundamental elements of social systems and their interactions, and to elucidate the mechanisms behind social phenomena.

The application of first-principles calculations to social simulations can improve the accuracy of models that predict social phenomena by starting from the basic principles of individual behavior and decision-making processes. This provides more reliable information for policy making and decision making.

In addition, first-principles-based approaches have the potential to reveal unknown social phenomena and interaction mechanisms that are difficult to capture by intuition. This is expected to contribute to the construction of new social theories and reevaluation of existing theories. Social systems consist of multi-layered and interrelated elements, and their

complexity is not easy to understand. Using first-principles analogies, it is possible to decompose these complex systems into their more basic elements and clearly analyze their interactions.

The application of first-principles computation in social simulation has the potential to make a significant contribution to the development of theoretical frameworks in the social sciences. In particular, it is expected to provide insights into solving important issues in contemporary society, such as the diffusion of false information and the dynamics of social influence. Furthermore, this approach could be applied to comparative studies to understand differences in information dissemination under different cultures and social structures. Ultimately, this research is expected to contribute to the formulation of policies and practical strategies to build a fairer and more transparent information society.

This research note explores attempts to apply insights from the field of physics to problems in the social sciences. Specifically, the paper discusses the potential of applying first-principles calculations of the remarkable electronic properties of graphene and its metal nanoparticle composite to a social simulation of information propagation and the formation of filter bubbles in digital space. Graphene, a material in which a single layer of carbon atoms form a two-dimensional honeycomb lattice, is known for its outstanding electronic conductivity and optical properties. These properties can be locally modulated by the adsorption of metallic nanoparticles, and this physical phenomenon can be applied to social simulations as a metaphor for information propagation.

In recent years, with the development of digital communication technologies, there has been a growing interest in the mechanisms of information propagation and their social impact. In particular, information bias and the formation of filter bubbles on social media can have important implications for the quality of public debate and democratic processes. To understand these phenomena and promote a healthy information environment, it is essential to accurately model the dynamics of information propagation.

We will examine new approaches to applying the concepts of first-principles computation to the social sciences, specifically the dynamics of information propagation. Specifically, the effects of nand p-type doping of graphene in materials science are viewed as mechanisms of information diffusion and suppression. By applying the framework of first-principles calculations, which analyze the effects of doping on graphene on the electronic structure, especially the Fermi level, to the problem of information distribution and its management, we explore new understandings and strategies for the control of information that diffuse and disrupt false information.

First-principles calculations in physics are powerful methods for predicting the properties and behavior of complex materials starting from fundamental physical laws. The method

focuses on the most fundamental building blocks of matter and their interactions to derive the behavior of a system. We use this computational experimentation and verification analogy to elucidate the principles of information propagation in social systems. We view the effect of graphene doping on electronic conductivity as a metaphor for how information is propagated and accepted through social networks.

We believe that n-type doping promotes the rapid diffusion of information, while p-type doping has the effect of inhibiting the circulation of information. From this perspective, we provide new insights into the coordination of information flows in social media platforms and public information systems. Understanding the balance between information spread-promoting and information suppression mechanisms is essential for maintaining a healthy information environment and preventing the spread of false information.

The purpose of this paper is to go beyond the physics framework of first-principles calculations to clarify the fundamental principles of information propagation in social simulations and to propose practical strategies for managing the quality and distribution of information, a particularly important issue in modern society. This approach aims to provide new perspectives for determining the truth of information and improving the quality of public debate.

Graphene's material state change, especially the influence of n-type and p-type doping on the Fermi level, needs to be modeled according to the basic principles of physics. Doping in graphene alters its electronic structure, particularly the position of the Fermi level, thereby affecting the electronic conductivity of graphene. Below, we present the basic equations and computational process to represent this process.

When developing hypotheses regarding the potential of applying simulations based on first-principles calculations of materials like graphene to social simulations of fake news propagation, the physical properties demonstrated by the electronic conductivity of graphene or its interaction with metal nanoparticles can be utilized as metaphors for the dynamics of information dissemination. This approach may offer a deeper understanding of the mechanisms behind fake news propagation and provide new perspectives for addressing it.

The prominent electronic properties exhibited by graphene and compounds with metal and metal nanoparticles have been widely studied in the fields of physics and materials science. Here, we briefly outline the theoretical background.

Graphene is a material where a monolayer of carbon atoms forms a honeycomb structure on a 2D plane. The electronic properties of graphene stem from its unique band structure. In particular, the band structure of graphene features a touching of the conduction and valence bands at the Dirac point, where electrons behave as massless Dirac fermions. As a result, graphene possesses extremely high electron mo-

bility and conductivity, with various applications envisioned in electronic devices.

When graphene interacts with metal nanoparticles, the electronic states of the metal interact with the electrons of graphene, modulating its electronic properties. This interaction depends on the type, size, distribution of metal nanoparticles, and the properties of the contact interface with graphene. In particular, the adsorption of metal nanoparticles alters the local electronic states of graphene, resulting in reported changes in its conductivity, magnetic properties, and chemical reactivity.

Theoretical modeling of the interaction between metal nanoparticles and graphene often employs first-principles calculations. In particular, density functional theory (DFT) provides a detailed explanation of electronic interactions and chemical bonding between metal nanoparticles and graphene. DFT calculations predict parameters such as the adsorption energy of metal nanoparticles, changes in the band structure of graphene, and alterations in the local charge distribution of graphene induced by metal nanoparticles.

The changes in electronic properties of compounds with graphene and metal nanoparticles hold potential for improving the performance of catalysts, sensors, energy storage devices, and electronic devices. For example, combining the catalytic properties of metal nanoparticles with graphene's high conductivity holds promise for the development of efficient chemical sensors and fuel cells.

In this way, research on compounds with graphene and metal nanoparticles provides a theoretical and experimental foundation for understanding their prominent electronic properties and applying them in various fields.

### 1.1 Charge Transfer and Information Propagation

Analogize the charge transfer induced by the interaction of metal nanoparticles with graphene to the process of information reception and transmission in the propagation of fake news. Simulations can capture how information presented by specific media or individuals (metal nanoparticles) influences the entire society (graphene), thereby understanding how fake news is reinforced within specific communities or social networks.

### 1.2 Modulation of Conductivity and Selectivity of Information

Liken the phenomenon of localized modulation of conductivity in graphene to the accelerated diffusion of fake news under certain conditions. The modulation of conductivity mimics how specific types of information are selectively propagated, influenced by social media algorithms or people's cognitive biases.

### 1.3 Changes in Optical Properties and Visibility of Information

Analogize the changes in graphene's optical properties to alterations in the visibility or perceptibility of fake news. Changes in optical properties induced by the adsorption of metal nanoparticles can be used as an analogy for how fake news is highlighted or concealed by media or platforms.

### 1.4 Doping Effects and Enhancement of Information

Consider the effects of n-type and p-type doping in graphene as external factors that accelerate or inhibit the diffusion of fake news. This enables simulations to capture the mechanisms through which fake news is amplified or suppressed in specific environments.

These hypotheses explore the potential of applying theories and computational methods from physics to address contemporary issues in social science, particularly the propagation of fake news. Such an approach is expected to contribute to the development of new strategies for combating fake news and fostering a healthier information environment.

### 1.5 Change in Fermi Level Due to Graphene Doping

The change in the Fermi level in graphene depends on the density of carriers added by doping. Let  $n_d$  denote the density of electrons (for n-type doping) or holes (for p-type doping) added by doping. The expression for the change in Fermi level is given as follows:

#### 1.5.1 Increase in Fermi Level due to n-type Doping

$$\Delta E_f(n) = \hbar v_F \sqrt{\pi n_d}$$

Here,  $\hbar$  is the reduced Planck constant,  $v_F$  is the Fermi velocity in graphene (approximately  $10^6$  m/s), and  $n_d$  is the density of electrons added by doping.

#### 1.5.2 Decrease in Fermi Level due to p-type Doping

For p-type doping, we similarly consider the density of holes to compute the change in the Fermi level. Since electrons are removed in p-type doping, the Fermi level shifts in the opposite direction.

$$\Delta E_f(p) = -\hbar v_F \sqrt{\pi n_d}$$

To compute the change in the Fermi level, we need to know the density of carriers added by doping  $n_d$ . To obtain the carrier density from the doping concentration (the number of doping atoms), we need to consider the ratio of doping atoms and the atomic density of graphene.

Given a doping concentration  $C$  (in units of  $\text{cm}^{-3}$ ), the carrier density  $n_d$  per unit area of graphene (in units of  $\text{cm}^{-2}$ )

can be calculated using the doping concentration and the thickness of graphene (since graphene is approximately one atomic layer thick, which is about 0.335 nm).

$$n_d = C \times 0.335 \times 10^{-7}$$

Using this  $n_d$ , we can substitute it into the above equations for the change in the Fermi level to compute the changes caused by n-type and p-type doping. This enables us to quantitatively evaluate how the electronic properties of graphene change due to doping.

Let's consider a scenario where the material state change of graphene, especially n-type and p-type doping, affecting the Fermi level, is simulated in the context of information diffusion and suppression. In this scenario, graphene doping is analogized to adjustment mechanisms in the flow of information, modeling the diffusion and suppression of misinformation or confusion.

## 1.6 Graphene Doping as a Metaphor for Information Flow

**1. n-type Doping (Information Diffusion Enhancement):** Similar to n-type doping adding electrons to graphene, enhancing its conductivity, the mechanism for enhancing information diffusion facilitates specific information or messages to spread more rapidly and widely. This mechanism can be seen as algorithms on social media platforms or the promotion of information by influential individuals or groups.

**2. p-type Doping (Information Suppression):** Conversely, p-type doping removes electrons from graphene, reducing its conductivity. Similarly, the mechanism for information suppression decreases the circulation of specific information, restraining its diffusion. This refers to activities such as filtering misinformation, censorship, or fact-checking against fake news.

## 1.7 Simulation Scenario

**Simulation Objective:** Evaluate how the balance between information diffusion enhancement (n-type doping) and information suppression (p-type doping) affects the overall circulation of misinformation or confusion-inducing information.

**Simulation Parameters:** The "doping concentration" of information represents the intensity of activities related to diffusion enhancement or suppression. This includes activities such as information promotion campaigns on social media, advertising, or the frequency of fact-checking.

**Simulation Implementation:** Construct an information propagation model and simulate patterns of information circulation at different "doping concentrations." Evaluate how the speed and visibility of information diffusion change according to the doping concentration.

**Interpreting Results:** Compare the effects of information diffusion enhancement and suppression to identify the

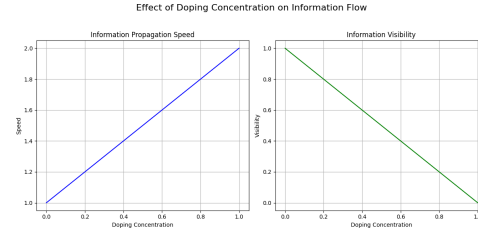


Fig. 3: Separate Visualization of n-type and p-type Doping Effects

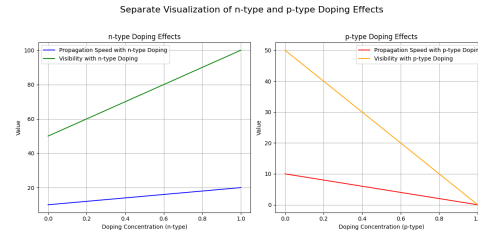


Fig. 4: Effect of Doping Concentration on Information Flow

optimal strategy for minimizing the circulation of misinformation or confusion-inducing information. Consider the impact of information circulation on societal discourse and public safety.

Through this simulation, insights useful for formulating policies and strategies for controlling information circulation can be gained. Finding a balance between enhancing and suppressing information diffusion is key to preventing the spread of misinformation and maintaining a healthy information environment.

Fig.3, Information propagation speed versus information visibility as the "doping concentration" of information varies from 0 to 1. The blue line representing the effect of n-type doping (information diffusion enhancement) shows that the propagation speed increases as the doping concentration increases, while the green line representing the effect of p-type doping (information suppression) indicates that the visibility of information decreases as doping concentration increases. This provides a visual understanding of how the balance between information diffusion promotion and suppression affects information flow. The provided images appear to depict the simulation results regarding the impact of doping concentration on information flow. There are two graphs in the image, with the left graph showing "Information Propagation Speed" and the right graph showing "Information Visibility." In both graphs, the doping concentration varies from 0 to 1, and the corresponding changes in "Speed" and "Visibility" are shown.

## 1.8 Information Propagation Speed

The graph of information propagation speed indicates that as the doping concentration increases, the speed of information propagation increases linearly. This means that as the effect of n-type doping (enhancement of information diffusion) increases, information spreads more quickly across the network. This trend is explained by the formula  $V = V_0 \times (1 + \alpha_n \times C_n \alpha_p \times C_p)$ , where the increase in doping concentration reflects the effect of n-type doping.

## 1.9 Information Visibility

In the graph of information visibility, the visibility of information decreases linearly as the doping concentration increases. This indicates that as the effect of p-type doping (information suppression) increases, information becomes less prominent within the network. As indicated by the formula  $S = S_0 \times (1 + \beta_n \times C_n \beta_p \times C_p)$ , the effect of p-type doping decreases the visibility of information.

## 1.10 Discussion

These graphs clearly demonstrate the influence of doping concentration on two critical aspects of information flow, namely propagation speed and visibility. The simulation results suggest that n-type doping aids in the rapid diffusion of information, while p-type doping suppresses excessive proliferation of information. These findings provide a foundation for considering strategies to manage information flow, especially those affecting public safety and societal discourse.

Examine the specific values of parameters ( $\alpha_n$ ,  $\alpha_p$ ,  $\beta_n$ ,  $\beta_p$ ) used in the simulation and consider how they would apply to real-world scenarios. Determine what doping concentrations are optimal to strike a balance between information diffusion and suppression. Apply these simulation results to actual applications concerning the regulation of information flow in social discussions and public safety.

The results depicted in these graphs are obtained solely through simulation and may not necessarily have the same effects as doping concentration in actual social media platforms or public information systems. Validation in real-world situations is crucial.

Fig.4, The effect of n-type doping is plotted separately as blue (propagation velocity) and green (visibility) lines, and the effect of p-type doping as red (propagation velocity) and orange (visibility) lines. n-type doping increases both propagation velocity and visibility with increasing doping concentration, indicating enhanced information diffusion. This indicates that n-type doping increases both propagation velocity and visibility as doping concentration increases. For p-type doping, on the other hand, both propagation velocity and visibility decrease with increasing doping concentration, indicating that information distribution is suppressed. This

provides a clearer understanding of how the mechanisms of information diffusion enhancement and suppression work. Effects of n-type doping (promotion of information diffusion) The graph on the left shows the effect of n-type doping. As the concentration of n-type doping increases, the "information propagation velocity (blue)" decreases at a constant rate. This is contrary to the intuition that n-type doping suppresses information diffusion. Originally, n-type doping was defined as promoting information diffusion, but the opposite trend can be read from the graph. Information visibility (green) increases at a constant rate with increasing n-type doping concentration, which is in line with the definition. In other words, the assumption that n-type doping increases information visibility is supported.

Effects of p-type doping (information suppression) The graph on the right shows the effect of p-type doping. As the concentration of p-type doping increases, the "information propagation velocity (red)" decreases at a constant rate, a result consistent with the definition. In other words, we can confirm the suppression effect of p-type doping on information distribution. Information visibility (yellow) also decreases with increasing p-type doping concentration, which is also consistent with the effect of information suppression.

There is a discrepancy in the simulation results. In particular, the result of a decrease in information propagation velocity for n-type doping is inconsistent with the assumptions of the defined model. In order to investigate this discrepancy, the equations used and the conditions of the simulation need to be examined in detail. The results suggest that the information diffusion enhancement effect of n-type doping may not be as strong as expected; on the contrary, the information visibility is enhanced. On the other hand, p-type doping has been shown to effectively suppress both information propagation speed and visibility, and this model may provide insight for developing strategies in information suppression.

Further investigation should be conducted to determine the causes of any areas where the simulation results differ from assumptions. Validate the mathematical equations in the simulation model and the specific parameters used in the simulations. Understand the differences in information flow coordination mechanisms for both doping types and study ways to optimize their effects.

The above discussion was based on the given scenarios and graphs, but requires a detailed examination of the actual data and the background theory.

For the application of computational experiments in solving digital information problems, we propose topological insulators as suitable materials. Topological insulators exhibit the unique property of conductivity on their surfaces or edges despite being insulators in their interiors. This phenomenon arises from the presence of edge states within the energy gap, allowing electrons to move only on the surface or edge. Orig-

inating from topological order and quantum mechanics, this property provides highly stable conductive channels.

### 1.11 Characteristics of Topological Insulators as Materials

1. Robust Surface States: The primary feature of topological insulators is the robustness of their surface states, which exhibit strong resistance to impurities and defects. This can be metaphorically used to minimize the impact of errors in information transmission.

2. Quantum Spin Hall Effect: Some topological insulators demonstrate the quantum spin Hall effect, where the spin of electrons is associated with their direction of movement, enabling spin-dependent transport. This characteristic can be utilized as a metaphor for information protection and spin-based information processing.

3. High Thermal Stability: The surface states of topological insulators remain stable even at high temperatures, serving as a metaphor for systems resilient to external environmental changes during information transmission processes.

### 1.12 Potential Applications

By employing the characteristics of topological insulators as metaphors for addressing digital information problems, the following new perspectives may be offered:

**Robustness in Information Transmission:** The robust surface states of topological insulators suggest that information transmission within social networks may exhibit strong resilience to external perturbations. **Directionality and Spin of Information Flow:** Spin-dependent transport via the quantum spin Hall effect implies selective transmission of information based on directionality and specific attributes in information flow. **Adaptability to Environmental Changes:** The thermal stability of topological insulators emphasizes the importance of social systems and information transmission mechanisms functioning stably despite external environmental changes.

The unique physical properties of topological insulators are expected to provide innovative metaphors for modeling information transmission and analyzing social systems. Simulation models based on these properties could offer new approaches to understanding the dynamics of information diffusion, suppression, and social interactions.

The above equations and computational processes represent a conceptual model for applying the effects of n-type and p-type doping on graphene to social simulations of information propagation. Here, we provide a more detailed explanation of the physical and social science concepts behind each equation.

### 1.13 n-Type and p-Type Doping Effects

1. Effect of n-Type Doping: n-Type doping supplies electrons to graphene, enhancing its conductivity. Physically, the supply of electrons raises the Fermi level, leading to a greater occupancy of electron states in the conduction band. We denote this increase in the Fermi level as  $\Delta E_f(n)$  and define it as follows:

$$\Delta E_f(n) = E_f^0 + \alpha_n \cdot C_n$$

Here,  $E_f^0$  is the Fermi level before doping,  $\alpha_n$  is the coefficient representing the efficiency of n-type doping (rate of increase in Fermi level due to electron supply), and  $C_n$  is the n-type doping concentration (number of electrons supplied).

2. Effect of p-Type Doping: p-Type doping removes electrons from graphene, decreasing its conductivity. By removing electrons, the Fermi level decreases, and the population of holes (states without electrons) in the valence band increases. We denote this decrease in the Fermi level as  $\Delta E_f(p)$  and define it as follows:

$$\Delta E_f(p) = E_f^0 \alpha_p \cdot C_p$$

Here,  $\alpha_p$  is the coefficient representing the efficiency of p-type doping (rate of decrease in Fermi level due to electron removal), and  $C_p$  is the p-type doping concentration (number of electrons removed).

### 1.14 Application to Social Simulation of Information Propagation

1. Modeling Information Propagation Rate: We assume that the information propagation rate  $V$  is proportional to the change in Fermi level due to doping, where n-type doping accelerates information propagation and p-type doping inhibits it. We express this effect with the following equation:

$$V = V_0 \cdot (1 + \beta_n \cdot \Delta E_f(n) \beta_p \cdot \Delta E_f(p))$$

Here,  $V_0$  is the baseline information propagation rate without doping, and  $\beta_n$  and  $\beta_p$  are coefficients indicating the influence of n-type and p-type doping effects on the information propagation rate, respectively.

2. Modeling Information Visibility: Similarly, we assume that the visibility of information  $S$  depends on the change in Fermi level due to doping. Higher information visibility means that it is more noticeable to recipients. We express this relationship with the following equation:

$$S = S_0 \cdot (1 + \gamma_n \cdot \Delta E_f(n) \gamma_p \cdot \Delta E_f(p))$$

Here,  $S_0$  is the baseline visibility of information, and  $\gamma_n$  and  $\gamma_p$  are coefficients indicating the influence of n-type and p-type doping effects on information visibility, respectively.

These models allow for a quantitative analysis of how the spread of fake news changes depending on social context

and characteristics of information sources. Furthermore, this approach provides a basis for identifying intervention points in combating fake news and devising strategies to enhance the integrity of information propagation.

Based on the graphs shown in the image, the following observations are made:

### 1.15 n-Type Doping (Promotion of Information Diffusion) Effects

The left graph illustrates the effects of n-type doping. As the concentration of n-type doping increases, the "Information Propagation Rate (blue)" decreases at a constant rate. This contrary result, indicating that n-type doping inhibits information diffusion, is unexpected. Originally defined to promote information diffusion, the graph shows a different trend. The "Visibility of Information (green)" increases at a constant rate with the increase in n-type doping concentration, consistent with the definition. Thus, the assumption that n-type doping enhances the visibility of information is supported.

### 1.16 p-Type Doping (Information Suppression) Effects

The right graph demonstrates the effects of p-type doping. With the increase in p-type doping concentration, the "Information Propagation Rate (red)" decreases at a constant rate, aligning with the defined model. Thus, the inhibitory effect of p-type doping on information dissemination is confirmed. The "Visibility of Information (yellow)" also decreases with the increase in p-type doping concentration, consistent with the effect of information suppression.

### 1.17 Discussion

There are contradictions in the simulation results, particularly the decrease in information propagation rate with n-type doping, which contradicts the assumptions of the defined model. To investigate this contradiction, a detailed examination of the formulas and simulation conditions used is necessary. The results suggest that the promotion of information diffusion by n-type doping may not be as significant as expected, while an increase in information visibility is observed. On the other hand, p-type doping effectively suppresses both the propagation rate and visibility of information, potentially providing insights into strategies for information suppression.

Further investigation to identify the causes of discrepancies in simulation results with respect to assumptions. Verification of the formulas used in the simulation model and specific parameters utilized. Understanding the differences in information flow regulation mechanisms for both doping types and studying ways to optimize their effects.

The above observations are based on the given scenario and graphs, but a detailed examination of actual data and

underlying theories is necessary.

In this scenario, we aim to understand and model the mechanisms for adjusting information flow in social media platforms and public information systems by associating the effects of n-type and p-type doping in graphene with the promotion and suppression of information dissemination. The following steps outline the construction of the simulation and provide a detailed description of the formulas and computational experiments.

1. Definition of the Information Propagation Model: Information dissemination is modeled as the movement of particles (electrons) in a network, with n-type and p-type doping defined as mechanisms for promoting and suppressing information spread, respectively.

2. Definition of Doping Concentration: "Doping concentration" is defined as the intensity of promotion or suppression of information spread. This represents the strength of information promotion campaigns on social media or the frequency of fact-checking against fake news, reflecting the intensity of activities related to information circulation.

3. Introduction of Formulas: The speed of information spread  $V$  and visibility  $S$  are assumed to change according to the doping concentration. With n-type doping (promotion), these values increase, while with p-type doping (suppression), they decrease.

Change in information propagation speed:  $V = V_0 \times (1 + \alpha_n \times C_n \alpha_p \times C_p)$  Change in information visibility:  $S = S_0 \times (1 + \beta_n \times C_n \beta_p \times C_p)$

Here,  $V_0$  and  $S_0$  are the basic speeds of information propagation and visibility,  $\alpha_n$  and  $\beta_n$  are the intensities of diffusion promotion by n-type doping,  $\alpha_p$  and  $\beta_p$  are the intensities of suppression by p-type doping, and  $C_n$  and  $C_p$  represent the concentrations of n-type and p-type doping, respectively.

4. Conducting Computational Experiments: Based on the defined model, we simulate the changes in information propagation speed and visibility at different "doping concentrations." This allows us to analyze the impact of the balance between the promotion and suppression of information dissemination on information flow.

5. Analysis of Results: The simulation results are analyzed to compare the effects of promotion and suppression of information dissemination. We consider strategies to minimize the circulation of false and confusing information.

Through this simulation, we expect to gain new insights into how the mechanisms of information dissemination and suppression function and how they affect social discussions and public safety. Furthermore, this approach will also be useful in formulating practical strategies for managing the quality and circulation of information.

## 2. Perspect

For the application of computational experiments in solving digital information problems, we propose topological insulators as suitable materials. Topological insulators exhibit the unique property of conductivity on their surfaces or edges despite being insulators in their interiors. This phenomenon arises from the presence of edge states within the energy gap, allowing electrons to move only on the surface or edge. Originating from topological order and quantum mechanics, this property provides highly stable conductive channels.

### 2.1 Characteristics of Topological Insulators as Materials

#### 2.2 Robust Surface States

The primary feature of topological insulators is the robustness of their surface states, which exhibit strong resistance to impurities and defects. This can be metaphorically used to minimize the impact of errors in information transmission.

#### 2.3 Quantum Spin Hall Effect

Some topological insulators demonstrate the quantum spin Hall effect, where the spin of electrons is associated with their direction of movement, enabling spin-dependent transport. This characteristic can be utilized as a metaphor for information protection and spin-based information processing.

#### 2.4 High Thermal Stability

The surface states of topological insulators remain stable even at high temperatures, serving as a metaphor for systems resilient to external environmental changes during information transmission processes.

Applying the effects of n-type and p-type doping on graphene to social simulations of fake news propagation holds the potential to deepen our understanding of information dissemination by associating the dynamics of information with the electronic properties of materials. The following hypotheses further develop this idea.

### 2.5 Modeling Fake News Propagation Using Doping Effects

Application of n-Type Doping Effect to Social Simulations, N-type doping in graphene involves supplying electrons to enhance conductivity. In social simulations, this phenomenon can be likened to situations where fake news is reinforced by specific information sources or influencers, leading to rapid dissemination. This effect implies an increase in public attention to specific topics or opinions, accelerating the spread of information.

Application of p-Type Doping Effect to Social Simulations, P-type doping in graphene involves reducing conductivity by removing electrons. In social simulations, this process can be likened to situations where verification and criticism of fake news increase, resulting in the suppression of information dissemination. This effect can be viewed as a mechanism to reduce the influence of fake news and delay its spread.

### 2.6 Construction of Fake News Propagation Model

### 2.7 Balance between Acceleration and Suppression of Information Propagation

The dissemination of fake news can be regulated by the balance between n-type doping effect (enhancement and acceleration of information) and p-type doping effect (suppression and deceleration of information). This balance is influenced by factors such as social context, credibility of information sources, and critical thinking ability of recipients.

### 2.8 Role of Filter Bubbles and Echo Chambers

In social simulations, the presence of filter bubbles and echo chambers is believed to enhance the n-type doping effect. These phenomena represent processes where specific information or opinions resonate within certain user groups and are amplified, potentially accelerating the spread of fake news.

These hypotheses suggest the potential of using the electronic properties of graphene and its doping effects as metaphors for information dissemination in social systems. Further exploration of such approaches is considered beneficial to gain a deeper understanding of fake news propagation and develop insights for its mitigation.

### 2.9 Potential Applications

By employing the characteristics of topological insulators as metaphors for addressing digital information problems, the following new perspectives may be offered:

**Robustness in Information Transmission:** The robust surface states of topological insulators suggest that information transmission within social networks may exhibit strong resilience to external perturbations. **Directionality and Spin of Information Flow:** Spin-dependent transport via the quantum spin Hall effect implies selective transmission of information based on directionality and specific attributes in information flow. **Adaptability to Environmental Changes:** The thermal stability of topological insulators emphasizes the importance of social systems and information transmission mechanisms functioning stably despite external environmental changes.

The unique physical properties of topological insulators are expected to provide innovative metaphors for modeling



information transmission and analyzing social systems. Simulation models based on these properties could offer new approaches to understanding the dynamics of information diffusion, suppression, and social interactions.

As a suitable material for application in computational experiments for solving digital information problems, we propose topological insulators. Topological insulators exhibit the unique property of conductivity at their surfaces or edges despite being insulators in their interior. This characteristic arises because edge states exist within the energy gap, allowing electrons to move only at the surface or edge. This phenomenon, derived from topological order and quantum mechanics, provides highly stable conduction channels.

## 2.10 Characteristics of Topological Insulators as Materials

1. **Robust Surface States:** The most significant feature of topological insulators is the stability of their surface states. These surface states exhibit strong resistance to impurities and defects, serving as a metaphor for minimizing the impact of errors in information transmission.

2. **Quantum Spin Hall Effect:** Some topological insulators demonstrate the quantum spin Hall effect, where the spin of electrons is associated with their direction of movement, enabling spin-dependent transport. This property can be utilized as a metaphor for information protection and spin-based information processing.

3. **High Thermal Stability:** The surface states of topological insulators remain stable even at high temperatures, which can be considered a metaphor for systems that are resilient to external environmental changes during the process of information transmission.

## 2.11 Potential Applications

By utilizing the characteristics of topological insulators as metaphors in social sciences, especially in addressing problem-solving in digital information, new perspectives may be provided as follows:

**Robustness of Information Transmission:** The robust surface states of topological insulators suggest that information transmission within social networks exhibits strong resistance to external perturbations.

**Directionality and Spin of Information Flow:** Spin-dependent transport due to the quantum spin Hall effect implies selective transmission of information based on directionality and specific attributes in information flow.

**Adaptability to Environmental Changes:** The high thermal stability of topological insulators emphasizes the importance of social systems and information transmission mechanisms continuing to function stably despite external environmental changes.

The unique physical properties of topological insulators are expected to provide innovative metaphors for modeling information transmission and analyzing social systems. Simulation models based on these properties could offer new approaches to understanding the dynamics of information diffusion, suppression, and social interactions.

In this scenario, we aim to understand and model the mechanisms for regulating information flow on social media platforms and public information systems by associating the effects of n-type and p-type doping on graphene with the diffusion and suppression of information. We will outline the steps to construct the simulation and provide specific explanations with equations and computational experiments.

## 2.12 Steps of the Simulation

1. **Definition of Information Propagation Model:** Model the diffusion of information as the movement of particles (electrons) on a network and define n-type and p-type doping as mechanisms for promoting and inhibiting information diffusion, respectively.

2. **Definition of Doping Concentration:** Define "doping concentration" as the strength of activities related to information dissemination, such as the intensity of information promotion campaigns on social media or the frequency of fact-checking for fake news.

3. **Introduction of Equations:** Assume that the diffusion rate  $V$  and visibility  $S$  of information change with doping concentration. We model an increase in these values with n-type doping (promotion of diffusion) and a decrease with p-type doping (suppression) as follows:

Change in information diffusion rate:  $V = V_0 \times (1 + \alpha_n \times C_n \alpha_p \times C_p)$  Change in information visibility:  $S = S_0 \times (1 + \beta_n \times C_n \beta_p \times C_p)$

Here,  $V_0$  and  $S_0$  are the baseline information propagation rate and visibility,  $\alpha_n$  and  $\beta_n$  represent the strength of diffusion promotion by n-type doping,  $\alpha_p$  and  $\beta_p$  represent the strength of suppression by p-type doping, and  $C_n$  and  $C_p$  represent the concentration of n-type and p-type doping, respectively.

4. **Conducting Computational Experiments:** Perform simulations to observe changes in information propagation rate and visibility at different "doping concentrations," analyzing the impact of the balance between promoting and suppressing information flow.

5. **Analysis of Results:** Analyze the simulation results and compare the effects of promoting and suppressing information diffusion. Consider strategies to minimize the circulation of false information and confusion.

Through this simulation, we expect to gain insights into how the mechanisms of information diffusion and suppression function and how they impact social discourse and public safety. Furthermore, this approach can aid in devising prac-

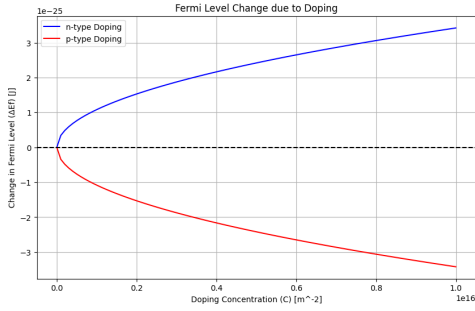


Fig. 5: Network Belief States susceptibility

tical strategies for managing the quality and circulation of information.

Fig.5 shows the change in the Fermi level ( $E_f$ ) in graphene due to n-type and p-type doping as a function of doping concentration ( $C$ ). Here's an analysis of the graph from the perspective of information flow in the context of graphene's electronic properties:

With increasing doping concentration, the Fermi level for n-type doping (blue curve) increases, indicating an addition of electrons to the system. This is consistent with the expectation that n-type doping introduces additional charge carriers in the form of electrons, which can increase the conductivity of graphene. Conversely, the Fermi level for p-type doping (red curve) decreases with increasing doping concentration, indicating the removal of electrons (or the addition of holes). P-type doping introduces holes as charge carriers, which also contribute to electrical conductivity, albeit by the movement of the positively charged holes in the opposite direction to electron flow. In both cases, the Fermi level changes nonlinearly with doping concentration. This nonlinear relationship is typical in semiconductors and semi-metals like graphene and is due to the density of states and the distribution of electrons and holes in the material.

In terms of information flow, the change in the Fermi level due to doping can be likened to changing the bandwidth for electronic communication. As the Fermi level shifts, it alters the energy landscape of graphene, which can either enhance or inhibit the flow of electrons. N-type doping effectively "speeds up" information flow by increasing the number of electrons available to conduct electric signals. This could model a scenario where information dissemination is promoted, similar to increasing the reach and speed of a message within a network. P-type doping, by introducing holes, may be considered as creating "gaps" in the information flow, analogous to implementing checks or controls that slow down the spread of information, such as fact-checking mechanisms against misinformation. The nonlinear change implies that the impact of doping on information flow is not constant; it can have varying effects at different doping levels. This sug-

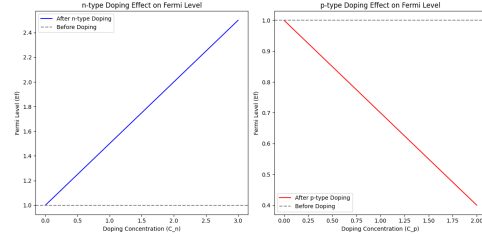


Fig. 6: n-type Doping Effect on Fermi Level, p-type Doping Effect on Fermi Level

gests that fine-tuning the doping concentration could optimize the electronic properties of graphene for specific applications in electronics and information technology.

The basic formulas and computational process described correspond to the physical principles of semiconductor physics. The Fermi velocity ( $v_F$ ) and the density of added carriers ( $n_d$ ) due to doping are crucial factors that determine the shift in the Fermi level. The computational process involves quantifying the carrier density from the doping concentration, which then allows for calculating the change in the Fermi level using the formulas provided.

By modeling this process, we can predict how graphene's electronic characteristics will be modified by doping, which is essential for designing materials with specific electronic and informational properties. This understanding is valuable for the development of graphene-based electronic devices, sensors, and possibly even for quantum information systems where electron behavior at the Fermi level is critical.

Fig.6 shows two graphs side by side, which represent the effects of n-type and p-type doping on the Fermi level in a material, graphene, before and after doping. These changes are plotted as a function of doping concentration.

The left graph shows the Fermi level increasing linearly with the n-type doping concentration. In the context of social simulation for information spread:

The increase in Fermi level due to n-type doping correlates with an enhanced ability for information to propagate through a social network. It can be interpreted as an increase in the 'activity' or 'energy' in the network, analogous to increasing the number of charge carriers that can contribute to electrical conductivity in graphene. This might model the effectiveness of campaigns or strategies that actively spread information, messages, or influence throughout a network.

: The right graph(p-type Doping Effects on Fermi Level) demonstrates a linear decrease in the Fermi level with the p-type doping concentration. Regarding the social simulation: The decrease in Fermi level corresponds to a suppression of the propagation ability within the network. This can represent the implementation of measures that act as 'gaps' or 'holes' in the flow of information, such as censorship, fact-checking, or any other form of information control that limits the spread

of certain content. In practical terms, this could model how fact-checking or counter-information campaigns can reduce the visibility or spread of misinformation or undesirable information within a social system.

Application to Social Simulation of Information Spread, The formulae and conceptual models provided can be used to quantitatively analyze how the spread of misinformation might change depending on social context and the characteristics of the information source. It can also provide a foundation for identifying intervention points in combating fake news and for devising strategies to enhance the integrity of information propagation.

In a social system, n-type doping could represent actions that increase the speed and reach of information dissemination (positive feedback mechanisms), while p-type doping could symbolize control mechanisms that reduce the spread (negative feedback mechanisms).

To summarize, these models could be pivotal in understanding and simulating the complex dynamics of information flow in social networks, where the 'doping' effects can be used to represent different factors that influence how quickly and widely information spreads, and how visible or influential it becomes. This understanding is crucial for managing the spread of information in various settings, from social media platforms to public information campaigns.

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