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An Ab-initio Study of the Electronic and Optical Properties of 3d Transition Metals doped Germanene

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ABSTRACT

Density Functional Theory (DFT) computations have been used to look into the electrical and optical characteristics of 3D Germanene sheets doped with transition metals (TM). Recent years have seen a major increase in interest in germanene, a two-dimensional allotrope of germanium, due to its potential use in electrical and optoelectronic devices. The effect of doping Germanene with several 3d TMs, such as titanium (Ti), vanadium (V), chromium (Cr), manganese (Mn), iron (Fe), cobalt (Co), nickel (Ni), and copper (Cu), on its structural, electrical, and optical properties is examined in this paper. In order to comprehend the structural stability and geometry of the systems, we first tune the lattice parameters and atomic locations of the doped Germanene sheets. To further evaluate the alteration of electronic characteristics brought on by TM doping, we compute the electronic band structures, density of states, and charge density distributions. Our findings point to major changes in the electronic band structures that have resulted in the creation of novel electronic states within the band gap and point to possible semiconductor device applications. In addition, we investigate the complicated dielectric function, refractive index, and absorption spectra of TM-doped Germanene. When compared to pure Germanene, the optical properties show significant changes. This suggests that the material's optical response can be tuned, which is important for optoelectronic devices like photodetectors and modulators.

Keywords : Germanene, Transition metal doped Germanene, Density Functional Theory

I. INTRODUCTION

Graphene has gained prominence across all scientific disciplines since its discovery in 2004 [1-4]. The electronics industry has conducted substantial research on germanene and a comparable 2D material [5]. The bond length between germanene and germanene is significantly longer than the bond length between carbon and carbon, and the bonding in silicon is formed via mixed sp2 and sp3 hybridization [6-8]. Germanene is superior to graphene in a number of key ways, including easier valley polarization, increased fitness, significantly higher spin-orbit coupling, and a better adjustable band gap [9]. Germanene has been identified as the best contender for a variety of applications, including the electrode of ion batteries [10-11], solar cells, chips, medicine [12], super capacitors [13], spintronics [14-16], and hydrogen storage. Two-dimensional materials have been a focal point of research and development in the quest to harness innovative materials with remarkable electrical and optical capabilities [17]. Germanene, a two-dimensional honeycomb lattice made of germanium atoms, is one of these materials that has drawn a lot of interest because of its distinct electrical structure and prospective uses in nanoelectronics and optoelectronics [18]. Additionally, the carefully regulated addition of transition metal dopants to such materials has created new opportunities for augmenting and customizing their electrical and optical properties [19-21]. When introduced into two-dimensional materials, transition metals, especially those from the 3d series, display exceptional electrical and magnetic capabilities. Their presence may result in changes to the host material's band structure, electronic density of states, and optical sensitivity [22]. Designing practical nanodevices and expanding our understanding of fundamental quantum events depend critically on our ability to comprehend the effects of 3d transition metal doping on germanene's electrical and optical characteristics [23]. A potent computational technique for examining the electrical and optical characteristics of materials at the atomic and molecular level is density functional theory (DFT) [24]. By solving the Schrödinger equation self-consistently, taking into account the electron-electron interactions and exchange-correlation effects, it enables a thorough understanding of the electronic structure and optical properties. DFT-based research is now crucial for understanding the complex behavior of doped two-dimensional materials [25].

The optoelectronic industries use germanene extensively as well [26]. When Rita John et al. investigated silicene from the IR to the far UV, they discovered that it is present in the IR and visible spectrums. Because the peaks in mono-vacancy silicene are moved to lower energies, DFT calculations revealed that it has two wider peaks than pure germanene [27]. Theoretically, strain engineering has been studied in tailoring the electronic and optical characteristics of single-layer silicene under mechanical strains [28]. Theoretically, the electrical and optical characteristics of metals in the third transition were examined for graphene [29]. For all of them, excellent improvements in static dielectric constant and remarkable reflectivity at low optical energy were observed. For ten transition metals doped SnO2 nanosheets, the intensity of reflection, refraction, and absorption is enhanced in the visible light range, and the absorption displays a red shift for Ni, Fe, Mn, and Cr doped germanene.

In this article, we examine the structural and electrical characteristics of germanene in its natural state and germanene that has been doped with transition metals: Fe and Zn. With this kind of doping, we compute the dielectric function and refractive index in order to compute several optical properties, such as reflectivity, electron loss function, absorption, optical conductivity, and reflection.

Computational Details: All the Ab-initio calculations of Ge and transition metal doped germanene are performed by Quantum Espresso simulation package within the density functional theory (DFT) framework [30]. The generalized gradient approximation (GGA)+Hubbard U parameter is used to determine the exchange-correlation potential using the Perdew-Burke-Ernzerhof (PBE) functional [31]. Different values of U were used in the calculations (U Fe=4, and U Zn=5). To estimate the interaction potential between the valence electrons and ionic core plane augmented wave (PAW) is used. The kinetic energy cut-off of 80 Ry and the charge density cut-off of 320 Ry are used throughout the computations for the plane wave. The Broyden-Fletcher-Goldfard-Shanno (BFGS) algorithm was used to do the geometrical optimization of Germanene and Transition metal doped Germanene [32]. The structure was relaxed when the forces were less than 0.001 eV/A and the total energy criterion was set at1 ×10–5 eV. In order to create the k-points for the irreducible Brillouin zone sampling for the geometrical optimization and electrical characteristics of the doped and pure germanene, a set of 7×7×1 Monkhorst-pack grids were utilised, and a denser grid of 13×13×1 was used for the density of states (DOS). Additionally, we added a 15 vacuum to prevent the periodic interaction in the z-direction.

Structural and Electronic Properties: The initial step in each system's optimization procedure is to reduce its energy consumption in order to identify its most stable condition. The optimum Ge-Ge bond length, Ge-Ge-Ge bond angle, lattice constant, and buckling height for pure germanene were calculated to be 2.26, 115.71°, 3.83, and 0.47, respectively [33].

Our calculation for pure germanene agrees well with earlier conclusions derived from DFT simulations. Fig. 1. depicts the structures in their optimal states, both unpolluted and doped [34]. In the Ge-Fe, Ge-Zn bond lengths, bond angles, lattice constants (a), local bulking (hz), total magnetic moments per supercell, magnetic moments contributed from 3d-transition metals, and magnetic moments contributed from the sum of all Ge atoms are shown as structural and electronic properties of doped germanene [34]. Atomic radius decreases from Ti to Zn, although the length of the bond (Ge-Fe and Ge-Zn) does not. The optimize lattice parameter after relaxation are $a = 8.10081$ and $c = 25.99336$ A^0.

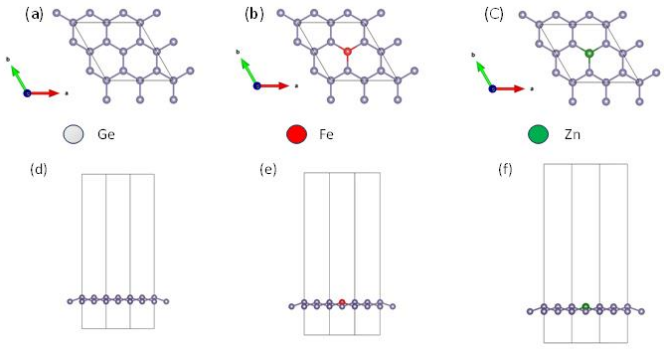

Fig.1. Shows that the (a) and (d) pure germanene, (b) and (e) Fe doped germanene, (c) and (f) Zn doped germanene along c and a direction respectively

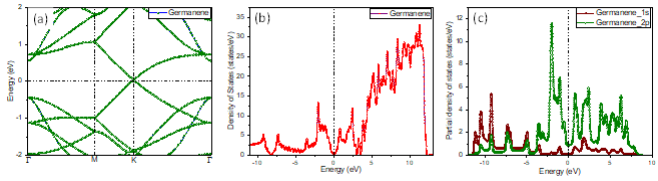

Fig.2. Shows that (a) band structure (b) density of states (c) partial density of states (PDOS) of germanene

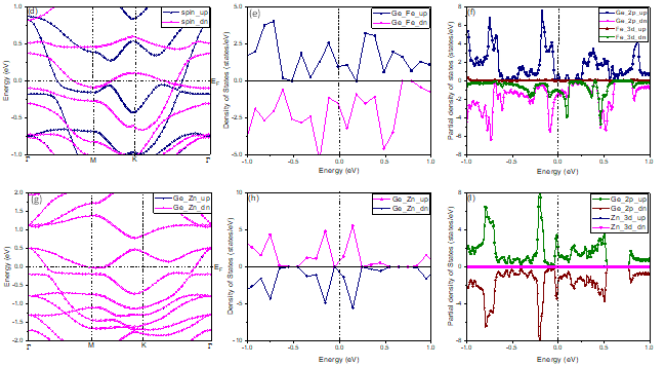

Fig.3. Shows that (d) band structure (e) density of states (f) partial density of states of Ge-Fe (g) band structure (h) density of states (I) partial density of density of Ge-Zn.

The electronic properties play a vital role in the field of electronics and optoelectronics devices [35]. Fig. 2 (a) shows that the band structure plot along the high symmetry point Γ→M→K→Γ by setting fermi energy at 0 eV. The density of states (DOS) and partial density of states (PDOS) are shown in Fig. (b) and (c). In fig (2) (c) it can be seen that the p orbital of the Ge atom dominated in the valence and conduction band region. Now, the band structure, DOS and PDOS transition metal doped germanene are shown in Fig. 3. In Fig. 3 (d), shows that spin up and spin down channel of band structure of Fe doped Ge. Similarly, DOS and PDOS are also shown in Fig. 3 (e). and (f). It can be seen that up spin of 2p orbital of Ge atom and down spin of 2p orbital of Ge atom are dominated in valence band region. Likewise, up spin of 2p orbital of Ge and down spin 3d orbital of Fe are dominated in the conduction band near the fermi energy range. Similarly, the band structure, DOS and PDOS of Zn doped germanene are shown in Fig. 3 (g), (h) and (I). In the band structure plot, it can be seen that the up and down spin of band are overlapped [36-38].

Optical Properties:

The optical characteristics of germanene that has been doped with transition metals- Fe and Zn have been estimated in this work [39]. We can learn about the dielectric function, refractive index, reflectivity, electron loss function, absorption, optical conductivity, and reflection from the optical properties. The optical characteristics of the Ge/GaAs heterostructure were estimated using the frequency-dependent complex dielectric function as follows:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \quad (1)$$

which is defined as the linear response of the medium to electromagnetic radiation. Where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are real (dispersive) and imaginary (absorptive) parts of the dielectric function, respectively. The imaginary part of the dielectric function is obtained by

$$\varepsilon_2(\omega) = \frac{2\pi e^2}{\Omega\varepsilon_0}\sum_{c,v,k}|\langle\varphi_k^c|\hat{u}\times\vec{r}|\varphi_k^v\rangle|^2\,\delta[E_k^c - (E_k^v + E)] \quad (2)$$

where the unit cell's volume is Ω, the electronic charge is e, the conduction and valence bands' wavefunctions are φ_k^c and φ_k^v, respectively, and the vector given by the polarisation of the electric field is u.

The real part of the dielectric function can be calculated from $\varepsilon_2(\omega)$, using the Kramer-Kronig relation [27].

$$\varepsilon_1(\omega) = 1 + \left(\frac{2P}{\pi}\right)\int_0^\infty \frac{\omega'^2\varepsilon_2(\omega')}{\omega'^2-\omega^2}d\omega' \quad (3)$$

The other optical parameters, such as Absorption coefficient $\alpha(\omega)$, Refractive index $n(\omega)$, and Optical conductivity $\sigma(\omega)$, can be estimated by calculating the real and imaginary part of the dielectric function [28].

$$\alpha(\omega) = \frac{\omega}{c}\sqrt{2\left(\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right)} \quad (4)$$

$$n(\omega) = \sqrt{\left(\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)} + \varepsilon_1(\omega)}{2}\right)} \quad (5)$$

$$\sigma(\omega) = \frac{\omega\varepsilon_2(\omega)}{4\pi} \quad (6)$$

The imaginary and real parts of the dielectric function are used to determine other optical constants such refractive index, reflectivity, electron loss function, absorption, optical conductivity, and reflection. The optical properties are described by the complex function known as the dielectric function [40]. It consists of two parts; the actual part refers to radiation photons scattered by materials, and the imaginary part has to do with the energy absorbed by those materials. Fig. 4. displays the real and imaginary curves of the dielectric function for pure germanene and doped germanene containing transition metals: Fe and Zn. When light is polarized in-plane (⊥), the real part of the dielectric function begins virtually at zero energy [41]. The value of static dielectric constant are 1.5, 1.6 and 1.5 for pure Ge, Fe doped Ge and Zn doped Ge respectively. The imaginary part of the dielectric function is directly related to the electronic band structure [42]. In figure 4(b), the edge (first critical points) of optical absorption of pure Ge, Fe doped germanene and Zn doped germanene occurs at 0 eV. This is related to the transition from the valance band maximum to conduction band minimum, which corresponds to the fundamental band gap and since the Ge, Fe doped germanene, Zn doped germanene has no optical edge, this corresponds to its metallic behaviour, which can be confirmed by electronic band structure plot shown in Fig. 2 and (3) (a).

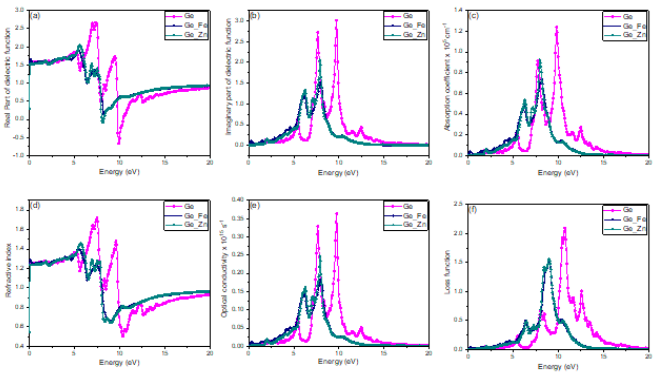

Fig. 4. Shows that (a) real part (b) imaginary part (c) absorption coefficient (d) refractive index (e) optical conductivity (f) Loss function of pure Ge, Fe and Zn doped germanene.

Absorption is a significant optical feature that, as we all know, is highly dependent on both the imaginary portion of the dielectric function and the direction of the light's polarization. In this study, we investigated the absorption of pure and doped germanene with transition metals under in-plane (⊥), the results are shown in Fig. 4 (c). The energy range was displayed as 0 to 20 eV. The maximal absorption peaks are 7.8, 7.9 and 10 eV in Fe, and Cu-doped germanene and pure germanene respectively [43].

How much electromagnetic radiation refracts after entering the material is indicated by its refractive index, n(ω). Fig. 4 (d) displays the refractive indices of pure germanene, Fe and Zn doped germanene. In good accord with experimental findings, the static refractive indices n(0) of pure germanene, Fe and Zn doped germanene are 1.26, 1.26, and 1.27, respectively [44]. Conductivity in the presence of an alternating electric field is known as optical conductivity. In Fig. 4(e), the germanene, Fe and Zn doped germanene optical conductivities as a function of frequency are shown. germanene, Fe and Zn doped germanene all exhibit increasing photoconductivity with energy, reaching maximum values at 7.8, 7.8, and 10 eV, respectively [45].

The electron energy loss function describes the energy loss of the fast-moving electron from the top of the valence band and the bottom of the conduction band. Fig. 4(f) depicts the electron energy loss functions of the pure germanene, Fe and Zn doped germanene [46]. The maximum value of the EELS spectrum for these pure germanene, Fe and Zn doped germanene, which are pure germanene, Fe and Zn doped germanene, is reached at 8.2, 8.3, and 10.3 eV, respectively. Plasma energy (_D) is the name for these materials' highest EELS peak. The real portion of the dielectric function disappears at the greatest point, demonstrating a sharp decline in reflectance [47].

II. CONCLUSION

In summary, DFT is used to ascertain the structural, electrical, and optical characteristics of the pure germanene, Fe and Zn doped germanene. Pure germanene, Fe and Zn doped germanene have computed band gaps of 0 eV. The optical characteristics, including the actual and fictitious components of the dielectric function, absorption coefficient, reflection coefficient, optical conductivity and EELS. The absorption spectrum demonstrates that these the pure germanene, Fe and Zn doped germanene have effectively absorbed light throughout a broad spectrum from 0.006 to 15 eV. The maximal absorption coefficients of pure germanene, Fe and Zn doped germanene are, respectively, at 7.8, 7.9 and 10 eV.

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