Structural, electronic and magnetic properties of Au-based monolayer derivatives in honeycomb structure

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Structural, Electronic and Magnetic Properties of Au-based Monolayer Derivatives in Honeycomb Structure

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Abstract. We present electronic properties of atomic layer of Au, Au_2-N, Au_2-O and Au_2-F in graphene-like structure within the framework of density functional theory (DFT). The lattice constant of derived monolayers are found to be higher than the pristine Au monolayer. Au monolayer is metallic in nature with quantum ballistic conductance calculated as $4G_0$. Similarly, Au_2-N and Au_2-F monolayers show $4G_0$ and $2G_0$ quantum conductance respectively while semiconducting nature with calculated band gap of 0.28 eV has been observed for Au_2-O monolayer. Most interestingly, half metalicity has been predicted for Au_2-N and Au_2-F monolayers. Our findings may have importance for the application of these monolayers in nanoelectronic and spintronics.

Keywords: DFT, monolayer, band structure, magnetic properties.
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INTRODUCTION

Two dimensional (2D) materials are nanoscale material with thickness ranging from 10nm-500nm. 2D materials possess unusual physical [1] and chemical properties [2] due to strong 2D quantum confinement and surface effects.

Gold in 2D form is receiving great attention with lots of promises for the next generation electronic applications e.g. interconnects in molecular circuits, sensors or devices for surface enhanced Raman scattering [3], biomedical applications and in plasmonics [4]. Various new materials can be derived by using 2D monolayers as building blocks [5]. Multilayer Au nanosheet are used as a stretchable electrodes for organic-based electronic devices [6]. They also find applications in displays, (FETs), nanodevices and energy-related devices [7].

The effect of defects and impurities on the electronic properties of graphene have been intensely investigated to tailor the band gap near the Fermi level in the last few years [8]. Similarly, SiGe-based 2D layered structures show diverse properties than their pristine counterparts [9].

In this paper, we show that the Au-based monolayer derivatives have distinctly different properties than the pristine form. Particularly, we. focus on the structural, electronic and magnetic properties of N-, O- and F-derived Au monolayers.

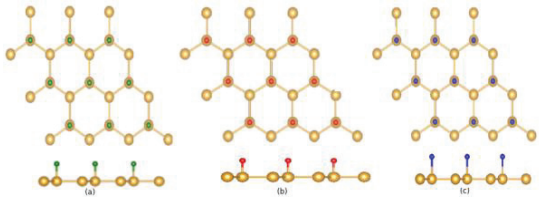

FIGURE 1. Top view and side view of (a) Au_2-N monolayer (b) Au_2-O monolayer (c) Au_2-F monolayer.

COMPUTATIONAL METHOD

All the calculations have been performed by using the SIESTA (*Spanish Initiative for Electronic Simulation with Thousand of Atoms*) code [10] and method which uses an ab initio pseudopotential based density functional theory (DFT). We have used well tested Troullier Martin, norm conserving relativistic pseudopotential in fully separable Kleinman and Bylander form. The exchange and correlation energies are treated within the generalized gradient approximation (GGA) according to the Perdew-Burke-Ernzerhof (PBE) parameterization [11]. Numerical atomic orbitals (NAOs) with double zeta polarization

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(DZP) basis set with confinement energy of 0.01 Ry have been used for geometry optimization. A 40x40x1 Monkhorst-Pack [12] of k points have been used for sampling the Brillion zone. The mesh cutoff energy has been taken equal to 200 Ry. A 16 A° vacuum to eliminate the interaction between the periodic images which ensures it to be isolated 2D monolayer.

RESULTS AND DISCUSSIONS

We have taken a fully relaxed Au-monolayer with 2 atom per unit cell in honeycomb lattice. Adding one of the atoms of N, O or F in 2D Au monolayer unit cell leads to Au_2-N, Au_2-O or Au_2-F periodic structures (Figure1). The fully relaxed configurations show graphene-like planer structure for all the considered systems. The calculated lattice constant of 2D pristine Au monolayer is 4.61 Å that increases to ~ 4.7 Å for its derivatives (Table 1). Similarly, binding energy of 2D Au monolayer is calculated as -2.24 eV/atom.

TABLE 1. The value of lattice constant a in Å, Au-N, Au-O, Au-F interatomic distance (d) in Å and binding energy per atom (E_b) in eV/atom..

System	a (Å)	d (Å)	E_b (eV/atom)
Au_2-N	4.72	1.99	-2.53
Au_2-O	4.71	1.82	-2.54
Au_2-F	4.69	2.15	-2.18

Note that the binding energy of the Au monolayer is calculated as

$$E_b = \left[E_{total} - nE_{Au}\right]/n$$

where E_{total} is the total energy of monolayer and E_{Au} is the total energy of the isolated Au atom and n is the number of atoms. The negative value of binding energy indicates the stability of the system. Similarly, The binding energy of derived Au_2X layer (X= N, O, F) are given as

$$E_b = [E_{total} - nE_{Au} - mE_X]/n + m$$

where E_{total} is total energy of Au_2X monolayer, E_{Au} the total energy of isolated Au atom, E_X is the total energy of isolated X (N, O, and X) atom, *n* and *m* represents the number of Au atoms and number of N, O or F atom. The binding energies of Au_2N and Au_2O monolayer are found to be higher than the pristine Au monolayer that results in to higher stability of Au_2N and Au_2O monolayer as compared to its pristine counterpart. Similarly, the Au_2F monolayer is energetically slightly less stable than pristine Au monolayer (Table 1).

Electronic and Magnetic Properties

It is observed from our spin polarized calculations that Au_2-N and Au_2-F structures are magnetic in nature in comparison with non-magnetic pristine Au monolayer. The magnetic moment is listed in Table 2. The magnetic behavior is also evident from the spin polarized density of states (Figure 2).

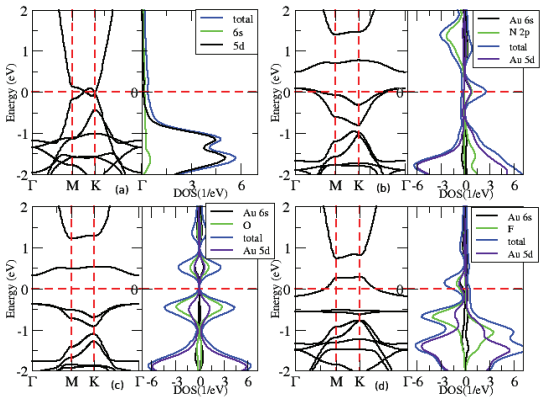

FIGURE 2. Electronic band structure and density of state for the monolayer of (a) pristine Au (b) Au_2N (c) Au_2O and (d) Au_2F. The Fermi level is set at 0 eV.

It is interesting to note that Au_2-N and Au_2-F monolayer shows zero states for one spin (up or down) and finite states for other spin (down or up) as can be seen in Figure 2 (b) and Figure 2 (d), that results into half metallicity in those systems. Half-metallic ferromagnets are seen as a key ingredient in future high performance spintronic devices because they have only one electronic spin channel at the Fermi energy. In case of Au_2-O monolayer, both spin up and spin down states are equal in magnitude indicating zero magnetic moment. It is inferred from the partial density of states that, not only Au but N, O and F atoms also show their contribution around Fermi energy.

TABLE 2. The values of magnetic moment and quantum ballistic conductance in case of Au- based monolayers.

System	Magnetic moment (μ_B)	Quantum ballistic conductance
Au_2-N	2.22	$4G_0$
Au_2-O	0	-
Au_2-F	0.87	$2G_0$

On analyzing the electronic band structure, we found that pristine Au-monolayer has four bands that cross the Fermi-level. Note that number of bands crossing the Fermi level gives the quantum ballistic conductance G_0. Therefore, quantum ballistic conductance of Au-monolayer is $4G_0$ which also

remains same for Au_2-N monolayers. In Au_2-F monolayers two bands are crossing Fermi-level, so it shows $2G_0$ quantum conductance. A small band gap about ~ 0.28 eV is calculated for Au_2-O monolayer.

CONCLUSIONS

In summary, electronic properties of Au_2-N, Au_2-O and Au_2-F monolayers are investigated within density functional theory. There is increase in lattice constant as we go from pristine Au monolayer to derived monolayers. Au_2-N and Au_2-F show half metallicity, while Au_2-O is semiconducting in nature. There is change in number of bands crossing the Fermi-level leading to variation in quantum ballistic conductance. These properties of Au monolayer and their derivatives suggest their potential use in tunable nanoelectronics and spintronics applications.

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