INTRODUCTION

Graphene is a one-atom-thick planar sheet of carbon atoms, which are ordered in hexagonal rings (honeycomb crystal lattice). In this work the geometric and electronic structure of graphene doped with gold atoms are calculated. The gold atoms are placed at three sites: H, B and T (see figures below). To find the structure with lower energy, the atoms positions are relaxed for each case. The band energy and density of states are calculated for the system with lower energy, and are compared with the calculated ones of pure graphene.

All the calculations were performed using the full potential augmented plane waves method with local orbitals (APW+lo) [1] within the framework of Density Functional Theory (DFT) [2], implemented in the computational code WIEN2k [3]. In the APW+lo method, the space is divided into an interstitial region and non-overlapping muffin-tin (MT) spheres centered at the atomic sites. This allows an accurate description of both the rapidly changing (oscillating) wave functions, potential and electron density close to the nuclei, as well as the smoother part of these quantities in between the atoms. Inside each of the MT spheres the wave function is expanded by a linear combination of radial wave functions multiplied by spherical harmonics, while in the interstitial region a plane wave expansion is used.

DENSITY OF STATES

The calculated density of states (DOS) of graphene and graphene-T are show below. The spin-up contribution is plotting with positive values, and spin-down with negative values. As can be seen from figures, the DOS contribution at Fermi level in graphene is null, and show a gap of 0.1 eV at Fermi energy, with similar spin-up and spin-down contribution in all range of energy values.

For graphene-T structure, the DOS contribution at Fermi energy is high. This density of states comes from s states of Au and p states of C, and C5, indicating an interaction between this atoms. The d states of Au are located far below the Fermi energy, not contributing to DOS at Fermi energy.

COMPUTATIONAL PARAMETERS

For relaxation of graphene with gold atoms at the three sites, we use a 5x5x1 k-mesh in the first Brillouin zone and R_{MT}K_{max}=5.0. For the relaxed structures, the calculations were performed with a 8x8x1 k-mesh and R_{MT}K_{max}=6.0. For the Density of States calculation, we use a more dense 16x16x1 k-mesh. For all calculations, the exchange-correlation potential was calculated within the Local Density Approximation (LDA) considering the spin polarization, with R_{MT} C=1.28 and R_{MT} Au=2.6.

REFERENCES


ACKNOWLEDGMENTS: R. Núñez-González is grateful to Área de Cómputo de Alto rendimiento de la Universidad de Sonora (ACARUS), for access to mezzite supercomputer system.

**RESULTS**

• The total energy analysis of the three structures show that the graphene with the gold atom at T-site is the most stable, with a energy difference of 0.024 eV with the graphene-B structure.
• From band energy and DOS calculation, Graphene-T is metallic with p states of carbon and s states of gold contributing at Fermi energy.
• At Fermi energy, the bands energy of spin-up and spin-down of graphene-T differ, specifically at K and M special k-point of Brillouin zone. This is observed in DOS figures as different intensities of density.
• At Fermi energy, the bands energy shown little dispersion, indicating the weak interaction between graphene and gold atom.

**ENERGY BANDS**

The calculated energy bands of graphene present the characteristic v-shape at Fermi energy level, touching the conduction and valence band at K special point. The spin-up and spin-down bands present the same shape.

Calculated energy bands of the low energy graphene-T structure show that the spin-up and spin-down bands are not equal for values near the Fermi energy, with bands crossing the Fermi level (conducting material). The low dispersion of the bands at Fermi level are indicating the weak interaction between graphene and gold atom.