Chemical stability of a new h-CuS monolayer – A DFT investigation.

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Abstract

The h-CuS monolayer has been investigated by means of density functional theory. It is derived from the covellite (CuS) and present structure similar to graphene. It is stable, non-magnetic and present metallic behavior. Multilayer structures have also been investigated.

Introduction

We investigated a copper sulfur (h-CuS) honeycomb sheet with similar structure of graphene. This structure was obtained by serendipity during the investigation of the covellite surface reconstruction. Figure 1 shows the (001) surface in which the h-CuS monolayer is formed due to covellite reconstruction and stabilized by van der Waals interactions with the surface. Due to its similarities to the graphene[1-3] and h-BN materials that are technologically important, we decided to investigate the properties and the stability of this material.

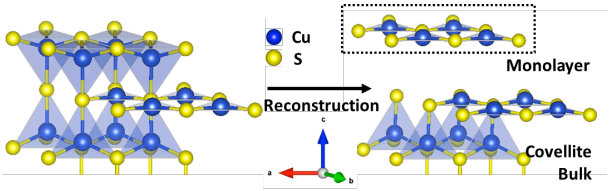

Figure 1. Fragment of covellite structure showing the reconstructions to form a monolayer.

Methodology

The electronic structures of the systems were calculated by GGA/PBE exchange/correlation approximation of the Density Functional method (DFT) as implemented in Quantum-ESPRESSO package. Following the Monkhost-Pack scheme 12x12x1 special k-points meshes were carry out for all slabs, and Kohn-Sham (KS) electronic orbitals were expanded in a plane-wave basis set up to a kinetic cutoff of 680 eV (50 Ry). Bader analysis was evaluated in CRITIC2 software. The h-CuS layer are placed in xy plane and modeled with a vacuum space of 15 Å in z-axis to avoid the interactions between two adjacent sheets.

Results and Discussion

Structural, electronic and mechanical properties were evaluated for the monolayer in vacuum, Figure 2a. The calculated Cu-S distances are 2.16 Å (0.04 Å less than in covellite) and the lattice parameter for the monolayer was determined to be **a=b=** 3.73 Å (0.1 Å less than in covellite). This observation is in a good agreement with Bader analysis, which observed that electron density increases in Cu-S BCP, suggesting stronger bond in the monolayer than in covellite bulk[3]. The system is non-magnetic, and the band structure (Figure 2b) indicated a metallic behavior of the monolayer. The projected Density of States (PDOS) shows that the conduction band is formed predominantly by p_x, p_y, $d_{x^2-y^2}$ and d_{xy} orbitals, suggesting that the conduction of the system occurs along xy plane, in the direction of the Cu-S bonds. It is in a good agreement with topological analysis, where all critical points (BCP and RCP, Figure 2a) is located in the sheet plane. Young modulus found by our theoretical level was 1406 GPa, a value greater than for graphene[3] (about 1000 GPa). The multilayer systems containing up to 5L-CuS monolayers was investigated. Preliminary results indicate that the 3-h-CuS is the most stable.

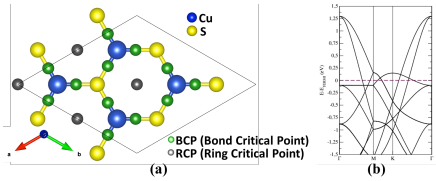

Figure 2. (a) Critical points analysis. (b) Band structure of the h-CuS.

Conclusions

A new two-dimensional stable material is proposed. The h-CuS has a metallic behavior with a high mechanical stability. Details about the 3L-CuS dynamical stability and its properties will be presented.

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