11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Systematic study of the electronic and structural properties of two dimensional semiconductors graphene-like structure

M. I. A. Oliveira(1)* and G. M. Dalpian(1)

(1) CCNH, Universidade Federal do ABC, Santo André-SP 09.210-170, Brasil
e-mail: maria.oliveira@ufabc.edu.br. * Corresponding author.

Abstract – The recent synthesis of the graphene shows that strictly two-dimensional crystals are indeed stable [1]. Besides, its high crystal quality makes of this a potential material for future devices. Theoretical and experimental studies have showed that not just the graphene can be stable and show interesting properties, but also other 2D materials such as the Si, Ge, ZnO and BN [2] can exhibit stable 2D graphene-like structure. In this work we present a systematic study of the electronic and structural properties of 2D semiconductors of type IV and type III-V, and we compare with those obtained for the *bulk* material.

Perfect two dimensional crystals were believed to be thermodynamically unstable until a few years ago. However, new theories and many experiments have been proving that these crystals can indeed exist [1]. Graphene, a single atomic plane of Carbon, has been recently synthesized and isolated, revealing an abundance of new physical properties and great potential for several technological applications. Besides Graphene, several different two dimensional materials are being studied both theoretically and experimentally. For example, ZnO nanosheets and 2D BN [2] have already been experimentally observed, whereas two dimensional Si and Ge (with graphene-like structure) have already been theoretically studied.

In this work, we will present a wide variety of results for most known semiconductor, but within the graphene-like structure. For this, we will perform *ab initio* calculations based on the Density Functional Theory and on the pseudopotential method. We will present the structural and electronic properties of type IV (C, Si and Ge) and type III-V (BN, GaAs and InN) semiconductors with graphene-like structure and compare their stability to their bulk counterparts (table 1). The same will be done for II-VI semiconductors, such as ZnO, ZnS, ZnSe and CdSe.

We have observed that most of these materials are semiconductors, but they are more stable in their bulk (zinc-blende or wurtzite) structures. Furthermore, a break in the symmetry of the lattice is observed due to the presence of different atomic species (figure 1), resulting in two different distances between the nearest neighbors (table 2).The next step of our work will consist on the study of 2D semiconductors of the type II-VI. Besides the differences of energies among the structures, we will also study the band structure of these materials.

Semiconductor	$\Delta E_{ZB\text{-}2D}$	*Semiconductor*	$\Delta E_{ZB\text{-}2D}$
AlAs	1.254	BP	1.033
AlN	1.271	InAs	1.209
AlP	1.275	InN	1.219
AlSb	1.234	InP	1.201
GaAs	1.167	InSb	1.183
GaN	0.981	SiC	1.290
GaP	1.142	SiGe	1.090
GaSb	1.188	Si	1.537
BN	0.169	Ge	1.281
C	0.063		

Table 1: Energy difference between 2D and *zinc blende* structures.

Semiconductor	d_1	d_2	*Semiconductor*	d_1	d_2
AlAs	2.329	2.327	BP	1.833	1.832
AlN	1.776	1.775	InAs	2.507	2.505
AlP	2.248	2.247	InN	2.053	2.051
AlSb	2.534	2.532	InP	2.432	2.430
GaAs	2.306	2.304	InSb	2.692	2.690
GaN	1.812	1.810	SiC	1.769	1.767
GaP	2.217	2.215	SiGe	2.268	2.266
GaSb	2.501	2.499	Si	2.230	
BN	1.430	1.429	Ge	2.326	
C	1.410				

Table 2: Distances between the nearest neighbors.

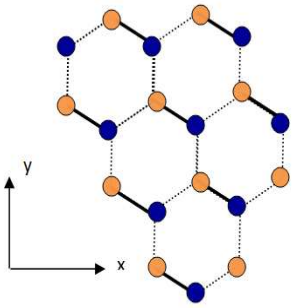

Figure 1: Break in the symmetry of the hexagonal lattice due to presence of different atoms. Distance represented by the full lines is larger than those represented by the stippled lines.

References

[1] A. K. Geim, and K. S. Novoselov, Nature Materials, 6 (2007) 183.
[2] C. Jin, F. Lin, K. Suenaga and S. Iijima, Physical Review Letters, 102 (2009) 195505.