A first principle study of the electronic states of hydrogenated \( \beta \)-SiC nanowires

A. E. Ramos\(^1\)*, M. Calvino\(^2\), and M. Cruz-Irisson\(^2\)

\(^1\)Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México
A.P. 70-360, 04510, D.F., México.
\(^2\)Instituto Politécnico Nacional, ESIME-Culhuacán, Av. Santa Ana 1000, 04430, D.F., México.

The study of luminescent properties of semiconductor nanocrystallites has been an active field of research since the first observation of strong photoluminescence of porous silicon at room temperature due to its potential applications as silicon-based visible-light-emitting devices integrated into microelectronics circuits. The development of low-dimensional semiconductor nanostructures has been the focus of research during the last two decades due to the changes in electronic and optical properties that occur when electrons are strongly confined in one, two, or three dimensions. In particular, one-dimensional silicon carbide (SiC) materials, i.e., nanowires are of great interest for many applications due to their excellent properties, such as high thermal conductivity and large band gap. In this work we have performed ab initio calculations on the structural and electronic band structure of the cubic (\( \beta \)) SiC nanowires by using the suite of programs Materials Studio, particularly using CASTEP, which is based on density functional theory. This study is carried out by means of a supercell technique \([1,2]\), in which along the [001] and [111] direction nanowires are constructed preserving the crystalline SiC atomic structure. The dangling bonds on nanowire surfaces are saturated with hydrogen atoms. A full geometry optimization is performed in order to lead the atoms to their minimal energy positions. The results show that the electronic states of cubic SiC nanowires depend strongly on their surface configurations and their crystallographic directions. Modifications of SiC nanocrystals surfaces may be a useful way to tune their electronic.

Keywords: Silicon Carbide, Nanowires, Electronic Structure, Ab-initio.


Acknowledgments: This work was partially supported by project CONACYT: 25231-F. The computing facilities of DGSCA-UNAM are fully recognized.

* eramos@iim.unam.mx