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AN ANALYTICAL STUDY ON THE LOCAL ELECTRONIC DENSITY OF STATES OF THE VALENCE BANDS IN AMORPHOUS SILICON CARBIDE

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A formulation for the energy-averaged local valence band density of states of amorphous silicon carbide is derived. To this end, sp^3-type hybrid orbitals are employed.

Keywords: Local valence band density of states; amorphous silicon carbide; hybrid orbitals

1. INTRODUCTION

Amorphous silicon carbide is a scarcely investigated material from both the theoretical and experimental points of view. However, some relatively recent research work has been developed; with respect to this, we refer to [1–3]. One of the open questions upon this semiconductor in the amorphous phase is related to the electronic density of states. In this paper, we shall propose a model for the evaluation of the energy-averaged local valence band density of states; in order to this estimation, molecular bonding orbitals will be employed.

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2. THEORY

It is well-known that the four tetrahedrally oriented bonds of a carbon atom are constructed from sp^3-type hybrid orbitals (see, for example, Ref. [4]). At this point, we will introduce the following orbitals [5]:

$$\phi_n = \psi_s + \sqrt{2}\,\psi_p \tag{1}$$

Now, also it is well-known that local density of states is given by:

$$g(\vec{r}, E) = \sum_n [|\psi_n(\vec{r})|^2 \delta(E - E_n)] \tag{2}$$

where δ and E denote delta Dirac's function and energy, respectively (for more details, see, for instance, Ref. [6]).

On the other hand, we can write [5]:

$$\psi_n = \sum_m [a_m \phi_n(\vec{r} - \vec{r}_m)] \qquad (n = 1, 2, \ldots, N) \tag{3}$$

Now, by combining formulae (1), (2) and (3), we get:

$$g(\vec{r}, E) = \sum_n \left\{ \left| \sum_m a_m [\psi_s(\vec{r} - \vec{r}_m) + \sqrt{2}\psi_p(\vec{r} - \vec{r}_m)] \right|^2 \delta(E - E_n) \right\} \tag{4}$$

By taking into account the structure of SiC molecules in the disordered phase (see, for example, Ref. [5]), we can claim that Eq. (4) is valid for valence bands. Then, under these conditions, it is feasible to write the following expression for the energy-averaged local electronic density of states, namely:

$$\langle g \rangle_E = \frac{1}{E_v} \int_0^{E_v} g(\vec{r}, E)\, dE \tag{5}$$

so that, by taking into consideration expression (4), from formula (5) it follows:

$$\langle g \rangle_E = E_v^{-1} \cdot N \cdot \left| \sum_m a_m [\psi_s(\vec{r} - \vec{r}_m) + \sqrt{2}\psi_p(\vec{r} - \vec{r}_m)] \right|^2 \tag{6}$$

3. CONCLUSIONS

We have obtained formula (6) as the main relationship of the above brief analysis. This study, although it is very brief, provides an interesting tool to examine more complex problems related to clusters in amorphous silicon carbide; at this point, in order to compute the total electronic density of states of relatively small clusters, taking Eq. (6) as starting point and with numerical calculations tangible results should be found.

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