Charge Transport in C60 Crystals: A Tight-Binding Description

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1. Introduction

Organic Semiconductors have attracted much attention since the discovery of their charge transport properties [1]. Unique features such as light weight and flexibility make them interesting for the electronics industry, particularly when new green energy solutions are considered. Since charge transport is the key step behind the performance of optoelectronic devices based in molecular crystals, a deep understanding about the charge carrier properties at a molecular scale is fundamental. Here, a numerical study is carried out to investigate the polaron transport in C60 crystals using a semi-empirical Holstein–Peierls model [2]. Importantly, the results presented here may throw new light on the description of the polaron properties in C60-based crystals.

2. Methodology

The model Hamiltonian adopted here considers both intra and intermolecular electron-lattice interactions for describing a two-dimensional array (single layer) of molecules [2]. Each molecule in the array is defined as a site i,j with three degrees of freedom: two antisymmetric non-local and phonon modes and one local phonon mode [2]. In our molecular array, the index j (x-direction) denotes the “columns” whereas i (y-direction) labels the “rows”. The model Hamiltonian adopted in this work -- that incorporates the Holstein and Peierls contributions in a single Hamiltonian -- follows the expression presented in the reference [2]. The set of model parameters, used to describe the C60 crystal, is originally developed in the present work.

3. Results

In our calculations, we have obtained for the polaron formation energy -- that represents the difference between the energies for systems in the neutral ground state and in a relaxed configuration due to the presence of an extra electron or hole -- a value about 50 meV, which lies in the range of values reported for other classes of molecular crystals [2]. Such a result indicates that the our set of model parameters can be describe the polaron properties for C60 crystals in a realistic fashion.

Regarding the charge carrier dynamics in the C60 systems, in our model, from the influence of external electric field, in a simulation 5 ps, the polaron moves approximately 25 Å from the origin, at a speed of approximately 5 Å/ps. The electric field used here has an intensity of 2.0 mV/Å. These results are presented in Figure 1.

Figure 1. Dynamics of Molecular Charge Density on a C60 Crystal.

3. Conclusions

The results showed that a suitable set of parameters, that is employed in our model Holstein-Peierls Hamiltonian, can play the role of distinguishing the properties related to the polaron stability and dynamics in different organic molecular crystals.

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5. References

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