Polaron Dynamics in Pentathienoacenes

^{1,*}Rayane Tayná da Costa Torres (PG), ²Marcelo Lopes Pereira Junior (PG), and ³Luiz Antônio Ribeiro Júnior (PQ)

¹University of Brasília, PPG-CIMA, Campus Planaltina, 73345-010, Brasília, DF, Brazil, ²Institute of Physics, University of Brasília, Brasília, 70910-970, DF, Brazil, ³International Center for Condensed Matter Physics, University of Brasília, P.O. Box 04531, 70.919-970, Brasília, DF, Brazil

¹rayane_torres27@hotmail.com ²marcelolpjuniorgmail.com ³ribeirojr@unb.br

Keywords: Charge Transport, Molecular Crystals, Polaron, Pentathienoacenes.

1. Introduction

Organic molecular crystals are now focus of attention due to their interesting properties in developing new green energy solutions [1]. Since charge transport is the key step behind the performance of devices based in molecular crystals, investigations to understand the charge carrier properties at a molecular scale is strongly desirable. In this way, here, a theoretical study is performed to investigate the polaron dynamics in Pentathienoacene crystals using a semi-empirical Holstein–Peierls model [2]. The present study is aimed at providing a nice description of the polaron properties in organic molecular crystals.

2. Methodology

The model Hamiltonian adopted here considers both intra and intermolecular electron-phonon interactions for describing a two-dimensional array of molecules [2]. Each molecule in the array possesses three degrees of freedom: two antisymmetric non-local and phonon modes and one local phonon mode [2]. The model Hamiltonian adopted in this work follows the expression presented in the reference [2]. The set of model parameters, used to describe the pentathienoacene crystal, is originally developed in the present work [3]. Figure 1 shows the Herringbone arrangement for the crystal and the directions considered by the tight-binding approach.

Figure 1. Herringbone arrangement for the pentathienoacene crystal.

3. Results

In our calculations, we have obtained for the polaron formation energy a value about 45 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 pentathienoacene crystals in a realistic fashion. On the other hand, pentathienoacene crystals have charge transport with one-dimensional characteristics, since the electron transfer integral in the *a*-direction (see Fig. 1) is 179 meV whereas in the *b* and *c* directions correspond both to 2 meV. Moreover, Figure 2 shows the dynamics of the charge carrier in Pentathienoacene crystals under influence of external electric field of 1.6 mV/Å. It is possible to note that, within this condition, the polaron saturation velocity is approximately 9 Å/ps.

Figure 2. Polaron dynamics in Pentathienoacene crystals.

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.

4. Acknowledgements

The authors gratefully acknowledge the financial support from the Brazilian Research Councils CAPES and FAPDF. L.A.R.J. gratefully acknowledges the financial support from the Brazilian Research Council FAPDF grant 0193.000942/2015 and 193.001.511/2017. L.A.R.J. also wishes to thank the Brazilian Ministry of Planning, Budget and Management (Grant DIPLA 005/2016).

5. References

- [1] V. Coropceanu, et. al. *Chem. Rev.*, **107**, 926-952, 2007.
- [2] L. A. Ribeiro and Sven Stafström. *Phys. Chem. Chem. Phys.*, **17**, 8973-8982, 2015.
- [3] E. Kim, et al. *Journal of the American Chemical Society*, **129**, 13072-13081.