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ORIGINAL PAPER

Polaron dynamics in oligoacene stacks

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Abstract The dynamical properties of polarons in organic molecular crystals are numerically studied in the framework of an one-dimensional Holstein-Peierls approach that includes lattice relaxation. Particularly, the present study is aimed at designing a tight-binding Hamiltonian that can address the charge transport mechanism in model oligoacene stacks. Our findings show that the definition of a particular oligoacene system depends strictly on the employed set of parameters. The usefulness of this methodology is highlighted by analyzing the polaron's saturation velocity and, consequently, its stability in the presence of a damping term and substantially high electric field strengths. Importantly, these results may be useful for the designing of novel materials to be employed in the field of molecular electronics.

Keywords Polaron dynamics · Organic molecular crystals · Oligoacenes

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Introduction

Organic semiconductors are considered so far the most promising materials for developing more efficient green energy applications [1, 2]. They have been successfully applied in the fabrication of flexible displays [3], transistors [4], and solar cells [5]. In all instances, these devices' performance critically depends on the efficiency with which charge carriers are transported within the organic material. In this material, the carriers responsible for mediating the charge transport are named polarons [6, 7]. Since the polaron transport is the key step behind the device's operation, when it comes to organic-based materials, a detailed knowledge about its dynamics in different molecular semiconductors may benefits the development of more efficient devices.

Oligoacene-based materials are widely used in the field of organic electronics mostly for presenting well-defined crystal structures [6]. Among them, pentacene (or pentacene-like) systems have been exhaustively employed in developing bilayer or bulk heterojunctions for optoelectronic applications [8]. Other oligoacene systems such as anthracene, naphtalene, tetracene, and rubrene have been also used in designing such applications [9–15]. The addition of substituents attached to aromatic rings of oligoacenes forms derivative materials that significantly improves the π-stacking interaction in the molecular crystal [16, 17]. This process makes the material quasi-one-dimensional with respect to the charge transport, leading the carrier to move primarily in the π-stacking direction [18–20]. Pentacene derivatives, for instance, may pack in three general motifs: slipped-stacks, columnar stacks, and segregated stacks [16]. Due its two-dimensional π-overlap, segregated stacks tend to exhibit the best device performance [16]. In this way, an

investigation that takes into account the polaron dynamics in one-dimensional oligoacenes becomes desirable.

It is well known that oligoacenes present two types of electron-phonon (e-ph) interactions, the local intramolecular (Holstein-type) and non-local intermolecular (Peierls-type). The last one takes place due to the weak intermolecular Van der Waals bonds presented by these materials [13]. Therefore, in order to describe these two types of e-ph interactions the Holstein and Peierls approaches should be incorporated in a single description, named Holstein-Peierls model [11]. The polaron dynamics in the presence of an external electric field, and in particular, time-domain Bloch Oscillations, have been extensively investigated by using one-dimensional tight-binding methodologies [21–25]. Particularly, some relevant studies have successfully addressed the polaron dynamics — in the framework of a Ehrenfest Molecular Dynamics — mostly in two-dimensional oligoacene materials by employing the Holstein-Peierls model [26–32]. However, recently, Y. Zhao and coworkers have developed a numerical exact method — named Dirac-Frenkel time-dependent variational approach with the Davydov *Ansatz* — where the accuracy of the simulated dynamics is significantly enhanced in comparison with the semi-classical Ehrenfest dynamics [25, 33–39]. Nonetheless, studies regarding the properties associated with the polaron dynamics in different molecular stacks (one-dimensional crystals) are very few in the literature and further investigations are needed.

In this work, a systematic numerical study is carried out to investigate the nonadiabatic polaron dynamics in different oligoacene systems by using a semi-empirical Holstein-Peierls model. An Ehrenfest Molecular Dynamics approach is carried out by considering an one-dimensional tight-binding model that includes lattice relaxation. The computational approach is based in defining model parameters that resemble molecular stacks of the following oligoacenes: naphthalene, anthracene, pentacene, tetracene, and rubrene. Importantly, the results presented here may provide guidance on the description of the polaron dynamics in strongly π-stacked oligoacene crystals.

Methods

The Holstein-Peierls Hamiltonian considered here includes both intra and intermolecular electron-lattice vibrations for describing an one-dimensional oligoacene crystal. Each molecule is represented for a site with two degrees of freedom: a local u_i and an antisymmetric non-local v_i phonon mode, as represented in Fig. 1. In this way, the model Hamiltonian assumes the following form

$$H = H_{elec} + H_{latt}, \tag{1}$$

where

$$H_{elec} = \sum_i \left[\alpha_1 u_i \hat{c}_i^\dagger \hat{c}_i + (J_{i+1,i}\hat{c}_i^\dagger \hat{c}_{i+1} + h.c.)\right]. \tag{2}$$

The first and second parts of H_{elec} considers the Holstein [40, 41] and Peierls [42–45] contributions, respectively. The operator $\hat{c}_{i,j}^\dagger$ ($\hat{c}_{i+1,j}$) creates (annihilates) an electron at the i-th molecule, α_1 is the intramolecular e-ph coupling and $J_{i+1,i}$ is the hopping term, which considers the intermolecular interactions in the form

$$J_{i+1,i} = J_0 - \alpha_2(v_{i+1} - v_i)e^{i\gamma A_x(t)}. \tag{3}$$

J_0 denotes the transfer integral in an uniformly spaced lattice and α_2 is the intermolecular e-ph coupling. The electric field is assumed to be static ans is included by using a time-dependent potential vector $A_x(t) = -cE_0t$, in which c is the speed of light and E_0 is the uniform field strength. $\gamma \equiv ea/\hbar c$ with e being the absolute value of the electronic charge and a the lattice constant.

The lattice backbone, in its turn, is described for two isolated harmonic oscillators

$$H_{latt} = \sum_i \left[\frac{K_1}{2}(u_i)^2 + \frac{M_1}{2}(\dot{u}_i)^2\right] + \sum_i \left[\frac{K_2}{2}(v_{i+1} - v_i)^2 + \frac{M_2}{2}(\dot{v}_i)^2\right], \tag{4}$$

Analogously to the electronic Hamiltonian, the first and second parts of H_{latt} describes the intra and intermolecular contributions, respectively. The index 1 refers to Holstein contribution whereas the index 2 denotes the Peierls contribution. K_1 (K_2) and M_1 (M_2) are the force constant and molecular mass for the intramolecular (intermolecular) phonon mode, respectively.

In some of our recent publications we have discussed in detail the methodology used to address the system dynamics, i. e., the Ehrenfest Molecular Dynamics [46, 47]. In particular, the electronic dynamics is governed by the time-dependent Schrödinger equation, which is solved using a propagator approach [46]. The lattice backbone dynamics, in its turn, is solved by employing the Euler-Lagrange equations, which are integrated in time using the Brünger-Brooks-Karplus integrator (BBK) [48]. The initial ground state configurations, which are the input for dynamical calculations, are obtained using the the Resilient backPROPogation algorithm (RPROP) [49].

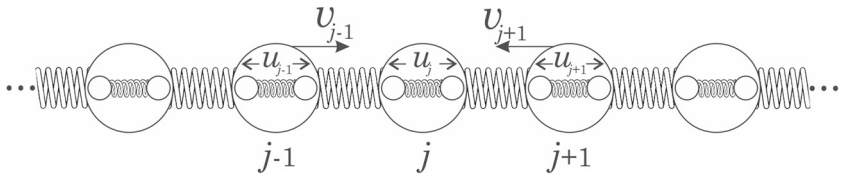

Fig. 1 Schematic representation of the model one-dimensional molecular crystal developed here. u_i and v_i are, the intra and intermolecular displacements for a given molecule, respectively

Since our model assumes a classical treatment for the lattice phonons, it is possible to make use of the Langevin approach to consider thermal effects. In this way, the temperature effects are simulated by adding thermal gaussian random forces with a zero mean value $\langle \zeta_n(t) \rangle \equiv 0$ and variance $\langle \zeta_n(t)\zeta_n(t') \rangle = 2k_B T\lambda M\delta(t - t')$. Normally, it is adopted a white stochastic signal $\zeta_n(t)$ as the fluctuation term. Furthermore, in order to keep the temperature constant at this initial value after a transient period (name thermalization), it is necessary to include a damping term λ. Therefore, the Newtonian equation of motion is modified according described in reference [46]. Here, we have introduced the dissipative force $(-\lambda\dot{v})$ and a gaussian random force $(\zeta_n(t))$ — that in the simulations performed here is assumed to be zero, i.e., no random fluctuations — in such a way to achieve the power spectral density given by the fluctuation-dissipation theorem.

The aim of the present work is to investigate the polaron dynamics in different one-dimensional oligoacene crystals by using a particular set of parameters for each system. The transfer integral values (J_0) considered here were successfully used in other theoretical studies [50–54] whereas the values for the intramolecular (Holstein) parameters α_1 and K_1 were obtained in calculations performed here. In these calculations, the values for the Holstein parameters have been chosen in order to obtain the minimal conditions to realize dynamically stable polarons for fixed intermolecular (Peierls) parameters $\alpha_2 = 0.5$ eV/Åand $K_2 = 1.5$ eV/Å, which are standard for modeling organic crystals when it comes to Holstein-Peierls models [11, 13, 30, 31, 46, 47]. The set of parameters defined for each system is presented in Table 1. It is worthwhile to mention that the modulation of the non-local parameters is strongly connected to external effects — such as temperature, pressure, and electric field — that may impact the molecular arrangement within the crystal. This arrangement is mostly governed by generally weak van der Waals intermolecular interactions. Once this particular kind of interaction not changes substantially among the pristine oligoacene crystals, the usage of same non-local parameters for all systems sounds as a reasonable approximation.

Results

We have pointed out above that this work is intended at describing the polaron dynamics in different molecular stacks, which are composed of oligoacene molecules. It may be instructive to begin our discussion by presenting the polaron motion in the presence of dissipation. The dissipation is considered by including a damping term λ (see reference [46]), which allows us to draw some conclusions about the temperature influence on the polaron dynamics. Here we have considered an one-dimensional lattice with periodic boundary conditions subjected to field strengths ranging from 2 up to 6 mV/Å. The polaron dynamics is accomplished during 5 ps. In this way, Fig. 2a and b display, respectively, the polaron dynamics in a pentacene stack for different damping strengths (for the sake of comparison with other studies) and the polaron dynamics in

Table 1 Set of parameters used in the simulations for each model oligoacene system

System	M_1 [eV(as/Å)^2]	M_2 [eV(as/Å)^2]	$J_0^{x,y}$ [meV]	α_1 [eV/Å]	K_1 [eV/Å^2]
Naphtalene	1.30×10^9	2.60×10^{10}	35.6	0.63	4.18
Anthracene	1.84×10^9	3.68×10^{10}	44.9	0.79	5.27
Pentacene	2.88×10^9	5.76×10^{10}	85.2	1.50	10.00
Tetracene	2.36×10^9	4.72×10^{10}	69.5	1.22	8.16
Rubrene	5.52×10^9	1.10×10^{11}	105	1.85	12.32

different oligoacene crystals for a certain damping value. In both cases, the electric field strength considered is 2.0 mV/Å. In Fig. 2a one can realize that the polaron motion (and consequently its velocity) is inversely proportional to the damping. This trend was also observed for the polaron dynamics in conjugated polymers [55]. In fact, for damping strengths ranging from 1.0×10^{1} to 1.0×10^{4} as^{-1} no differences in the polaron trajectory can be observed. It means that these damping strengths are substantially low in the sense that they can not be considered in studies where temperature effects are taken into account. Conversely, for damping values higher than 1.0×10^{4} as^{-1}, the polaron motion is considerably compromised in such a way that the polaronic charge can not flow for more than six sites for $\lambda = 1.0 \times 10^{6}$ as^{-1}, as can be seen in Fig. 2a. Once in molecular dynamics the temperature is normally modeled by including a fluctuation-dissipation term in the equation of motion by means of a Langevin formalism (as described in the previous section), one can conclude from results presented in Fig. 2a that the temperature effects leads to a damping in the polaron motion. Moreover, when it comes to modeling charge transport in crystalline organic semiconductors, it is clear that the minimal strength to realize a damping in the polaron transport should be $\lambda = 1.0 \times 10^{4}$ as^{-1}. Another interesting point is that even small strengths of λ can play the role of dissipate the polaron motion. Very recently, some studies have reported polaron velocities in one- and two-dimensional pentacene crystals ranging from

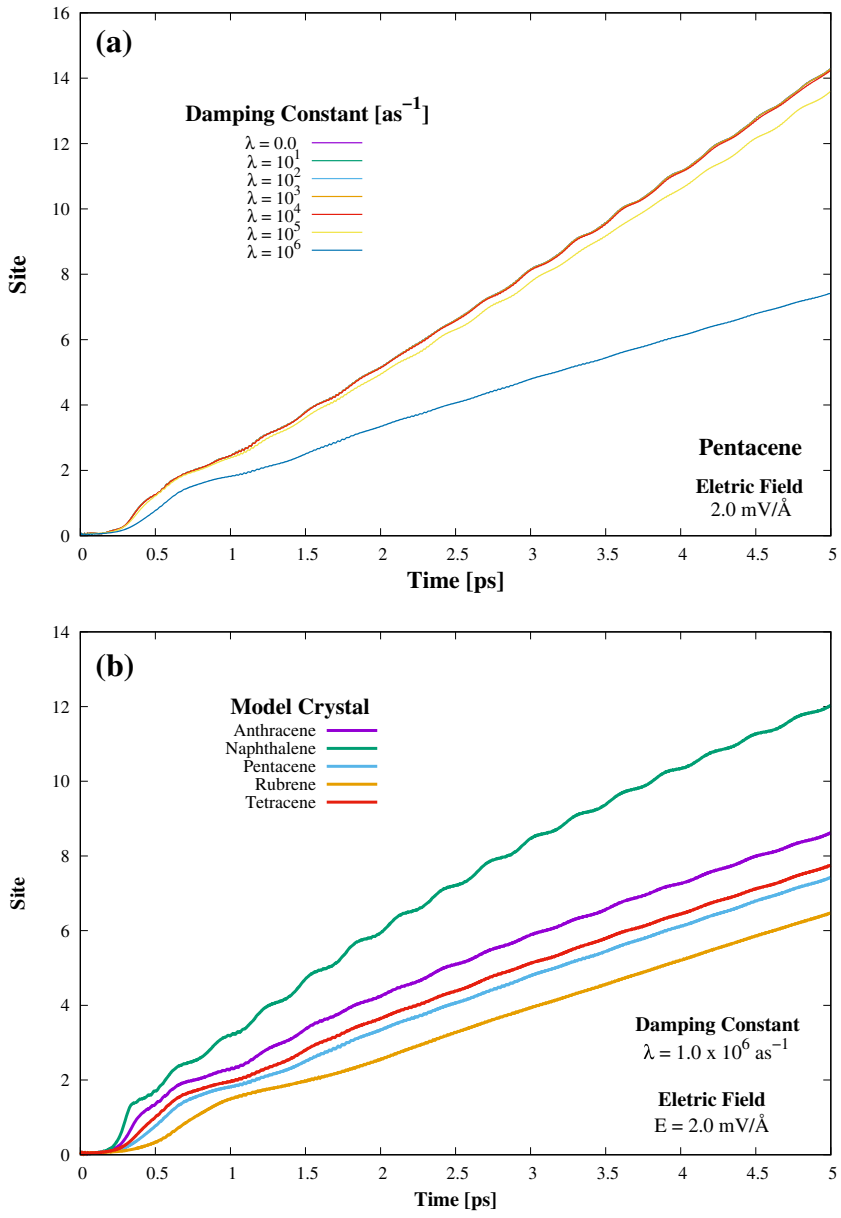

Fig. 2 The polaron's trajectory in different oligoacene stacks for an electric field strength of 2.0 mV/Åand for a damping constant of 1.0×10^{6} as^{-1}

12 to 20 Å/ps [31, 46, 47]. Here, by setting the lattice parameter (distance between next-neighboring sites) as 3.5 Å, the polaron velocity for λ values smaller than $1.0\times10^4\ as^{-1}$ is about 10 Å/ps, as can be inferred from Fig. 2a.

In order to realize the usefulness of our methodology at describing the polaron properties in one-dimensional molecular crystals, we now turn to the polaron's trajectory in different oligoacene systems for a field strength of 2.0 mV/Å and for a damping constant of $1.0\times10^6\ as^{-1}$, as displayed in Fig. 2b. The first interesting result that can be obtained from this figure is that the polaron motion is not strictly dependent of the transfer integral, instead, it depends of a suitable balance between the strengths of the intramolecular e-ph coupling and transfer integral. From Fig. 2b it is possible to note that the best relationship between J_0 and α_1 for the polaron dynamics is achieved when a naphtalene stack is considered. On the other hand, the rubrene stack shows the lowest covered distance for the polaron trajectory, which indicates — in the scope of our model Hamiltonian — that rubrene presents a considerably strong e-ph coupling strength for its intermolecular transfer integral. It is worthwhile to mention that after 5 ps the polaron trajectories increase almost linearly for all systems, once the electric field is not turned off.

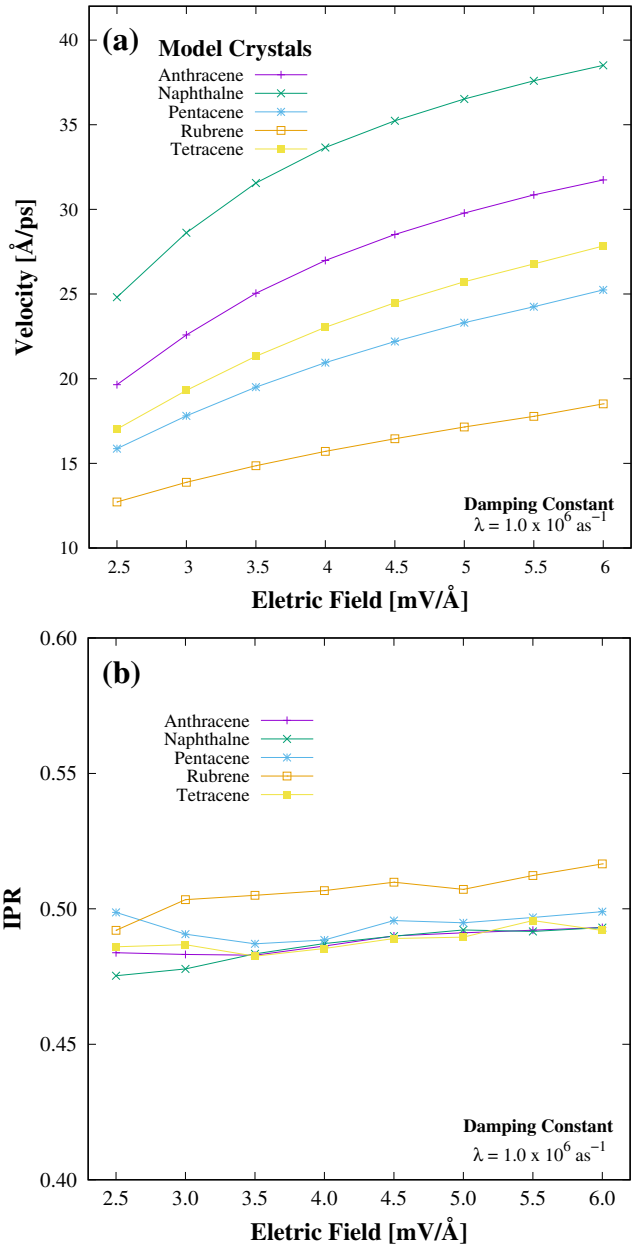

Fig. 3 **a** Polaron saturation velocities and **b** inverse participation ration (IPR) calculated for different oligoacene stacks subjected to electric field strengths ranging from 2.0 to 6.0 mV/Åand a damping constant of $1.0\times10^6\ as^{-1}$

Finally, we turn to the polaron saturation velocities obtained at each oligoacene system for field strengths ranging from 2.0 to 6.0 mV/Åand a damping constant of $1.0\times10^6\ as^{-1}$. In this way, from Fig. 3a one can realize that the same trend present in Fig. 2b is preserved, i. e., higher saturation velocities are achieved for naphtalene whereas the lower ones are obtained when rubrene stacks are taken into account. The remaining systems also preserve the trend displayed in Fig. 2b. Another clear feature is that, for field strengths higher than 4.0 mV/Å, the relationship between electric field and polaron velocity is linear. Interestingly, the polaron polaron keeps its stability even for high field strengths, i. e., for values higher than 3.0 mV/Å. An observable used to confirm that the polaron manages to keep its stability, even for high field strengths, is the inverse participation ration (IPR). Here we have used the time average value of IPR, calculated during the last picosecond of simulation, according established in the references [46, 47]. The average IPR is calculated only in the last picosencond in order to neglect the contribution of the ground state localization of the polaron. In this way, just its dynamical localization is taken into account. The average IPR values calculated for each field strength are displayed in Fig. 3b. In this figure one can conclude that in all situations the polaron keeps its integrity, once IPR values greater than 0.4 represent a stable polaron solution [46, 47]. It was recently reported that in two-dimensional oligoacene crystals, the polaron loses its integrity when fields strengths higher than this critical values are taken into account [46]. The results presented in Fig. 3 suggest that polarons are more stable structures in one-dimensional systems.

Conclusions

In summary, the nonadiabatic dynamics of polarons in different oligoacene systems is investigated in the framework of an one-dimensional Holstein-Peierls model that

includes lattice relaxation. Our results show that the polaron saturation velocity is inversely proportional to the damping constant, which in our discussion means temperature may acts in the system in order to suppress the polaron dynamics. Meanwhile, we find that the polaron's motion is not strictly dependent of the transfer integral, instead, it depends of a suitable balance between the strengths of the intramolecular electron-phonon coupling and transfer integral. We also show that, in the presence of a damping term, the threshold field that dissociates the polaron in two-dimensional systems is not strong enough to annihilate the polaron when it comes to its dynamics in one-dimensional systems, which suggests that polarons in molecular stacks are more stable structures than their analogous in two-dimensional molecular crystals. Albeit other approaches have been used to describe the polaron dynamics in organic molecular systems in a more accurate fashion, mostly the one that takes into account exact numerical methods [25, 33–39], our results provide, qualitatively, a consistent physical picture of the polaron dynamics in organic molecular crystals.

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