

Polaron transport in porous graphene nanoribbons

Wiliam F. da Cunha^a, Marcelo L. Pereira Júnior^{a,*}, William F. Giazza^b, Rafael T. de Sousa Junior^b, Luiz A. Ribeiro Júnior^{a,c}, Geraldo M. e Silva^a

^a Institute of Physics, University of Brasília, Brasília, Brazil

^b Department of Electrical Engineering, University of Brasília, 70919-970, Brazil

^c PPGCIMA, Campus Planaltina, University of Brasília, 73345-010 Brasília, Brazil

ARTICLE INFO

Keywords:

Polarons

Porous graphene nanoribbons

Charge transport mechanism

ABSTRACT

Porous graphene (PG) forms a class of graphene-related materials with nanoporous architectures. Their unique atomic arrangements present interconnected networks with high surface area and high pore volume. Some remarkable PG properties, such as high mechanical strength and good thermal stability, have been widely studied. However, their electrical conductivity, and most importantly, their charge transport mechanism are still not fully understood. Herein, we employed a numerical approach based on a 2D tight-binding model Hamiltonian to first reveal the nature of the charge transport mechanism in PG nanoribbons. Results showed that the charge transport in these materials is mediated by polarons. These carrier species are dynamically stable and present very shallow lattice distortions. The porosity allows for polaron-like charge carriers, and it can preserve the PG semiconducting character even in broader nanoribbons. The polarons move in PG within the optical regime with terminal velocities varying from 0.50 up to 1.15 Å/fs. These velocities are lower than those for polarons in conventional graphene nanoribbons (2.2–5.1 Å/fs).

1. Introduction

One of the most important goals of material engineering field is to conceive systems that combine the advantages of different materials for a given application [1–4]. For instance, the optical and mechanical properties of graphene sheets are very well established and celebrated [5,6]. However, this system lacks at least one crucial feature for its usage in optoelectronic devices, namely a finite bandgap [7–9]. The atomic-level control for structural modifications in the graphene sheet is arguably an option to give rise to related materials that present such desirable properties [10–13]. The search for systems based on graphene is the rationale behind the great effort in investigating materials of different symmetries [14–16]. As graphene, all those systems are solely composed of carbon atoms. Their distinct configurations are reflected in very different behavior as far as electronic properties are concerned [17–19]. Among them, Porous Graphene (PG) has been successfully synthesized [20,21] and presented a direct band gap in the range of 2.3–3.2 eV [22,21], which is of the order of what is desired for an organic semiconductor device [4,23–26]. Very often, polarons and bipolarons are responsible for the charge transport in graphene-based materials [27–29]. They are a product of the energetic interplay between the

electronic and the lattice degrees of freedom.

A usual procedure to obtain non-vanishing bandgap materials from graphene is to cut the sheet in narrow stripes of different widths and edges, thus yielding Nanoribbons [30–33]. The confinement effects of the wave function of the charge carrier in one dimension contribute to the arising of desirable properties from the mobility point of view [34–38]. The literature has dedicated some effort in the theoretical and experimental description of PG conducting properties in recent years [39–50]. Nonetheless, an investigation of the dynamics of the charge carriers in PG nanoribbon is still absent, even being crucial to the understanding of the transport properties of this system.

In this work, we studied the transport of charge carriers in PG nanoribbons by employing a two-dimensional lattice relaxation endowed Hamiltonian. To understand the time-dependent properties of the system, we conducted a time evolution of the degrees of freedom of both electrons and lattice parts of the system. The crucial issue addressed here concerns the very nature of the transport mechanism in PG nanoribbons. Based on our numerical approach, the findings revealed that polarons mediated the charge transport mechanism in PG nanoribbons.

* Corresponding author.

E-mail address: marcelolpjunior@gmail.com (M.L. Pereira Júnior).

<https://doi.org/10.1016/j.commsci.2021.110423>

Received 23 December 2020; Received in revised form 1 March 2021; Accepted 2 March 2021

Available online 9 April 2021

0927-0256/© 2021 Elsevier B.V. All rights reserved.

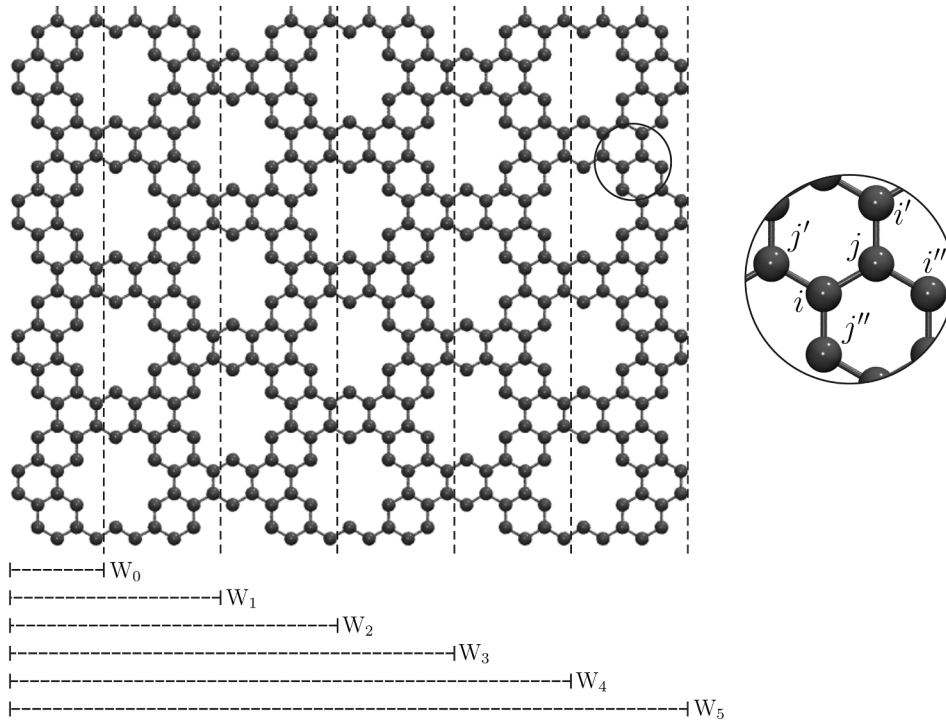


Fig. 1. Schematic representation of the PG nanoribbons studied in this work. Each dashed vertical line illustrates a nanoribbon of different width. The inset contains the labeling of the sites to be used in the model Hamiltonian. Note that the dashed lines are just representing the limit for a particular ribbon width. In this sense, no dangling bonds are formed by cutting the lattice.

2. Methodology

PG nanoribbons are obtained by periodically extracting carbon atoms from an armchair graphene nanoribbons. The left side of Fig. 1 represents a section of the resulting PG sheet, and the inset on the right shows the labeling of the sites to be used in the model. The dashed vertical lines represent PG nanoribbons of different widths. Note that these lines are just representing the limit for a particular ribbon width. In this sense, no dangling bonds are formed by cutting the lattice. The simulated systems have periodic boundary conditions in the vertical direction, as illustrated in Fig. 1.

To correctly address the interplay between phonons and electrons, we resort to a hybrid model that combines classical and quantum treatments. In this sense, we applied the second quantization formalism of quantum mechanics to treat the electrons and the Euler–Lagrange equations to treat the lattice [51]. These two realms are connected by an electron–phonon coupling term that includes lattice relaxation to an otherwise two-dimensional tight-binding model [52]. As is typical in sp^2 hybridized carbon systems, the displacement of the atoms in graphene is limited so that the electronic transfer integral for π -electrons can be expanded in first-order [27], thus resulting in hopping terms such as

$$t_{ij} = t_0 - \alpha \eta_{ij}. \quad (1)$$

In the equation above, t_0 is the hopping integral of a regular lattice, α the electron–phonon coupling, and η_{ij} are the variations in the bond-lengths of two neighboring sites i and j , as referred in the inset of Fig. 1.

Considering the aforementioned expression for the hopping term, the resulting Hamiltonian is expressed as

$$H = - \sum_{\langle i,j \rangle, s} (t_{ij} C_{i,s}^\dagger C_{j,s} + t_{ij}^* C_{j,s}^\dagger C_{i,s}) + \frac{1}{2} K \sum_{\langle i,j \rangle} \eta_{ij}^2 + \frac{1}{2M} \sum_i p_i^2, \quad (2)$$

where $\langle i,j \rangle$ means that the sum is performed over the neighboring sites labeled according to Fig. 1; $C_{i,s}$ ($C_{i,s}^\dagger$) is the π -electron annihilation (creation) operator on site i with spin s . The second term represents the

harmonic modeling of the effective potential associated with σ -bonds between carbon atoms, with K being the corresponding Hooke constant. As p_i and M are, respectively the atoms momentum and mass, the last term describes the kinetic energy associated to the sites. In a semi-empirical fashion we adopted the set of parameters most successfully reported in the literature: 2.7 eV for t_0 , 21 eV/Å² for K , and 4.1 eV/Å for α [53–59].

By beginning from a given initial set of coordinates $\{\eta_{ij}\}$, a self-consistent stationary solution (with $p_i = 0$) of the system is determined as follows: The ground state corresponding to the set $\{\eta_{ij}\}$ is obtained by diagonalizing the electronic Hamiltonian. The procedure also results in the determination of the eigenenergies of the system. From such states, it is possible to obtain the expected value of the system's Lagrangean. This operator is then used in Euler–Lagrange equations, and a new set of coordinates is accordingly obtained. A new iteration takes place when one uses the new set of coordinates to write a new Hamiltonian. The convergence criteria are observed by comparing the variations in the corresponding system's $\{\eta_{ij}\}$ and $\{\psi_{k,i,s}\}$ between consecutive iterations. The procedure can be characterized as an auto-consistent calculation in which the set of coordinates $\{\eta_{ij}\}$ is associated to the electronic set $\{\psi_{k,i,s}\}$ [51].

Crucial to this work is the time evolution of the system. As our model is hybrid, although a coupled one, time dependence of the electronic part is performed differently from that of the lattice. For the electrons, the time-dependent Schrödinger equation is used,

$$|\psi_k(t+dt)\rangle = e^{-\frac{i}{\hbar} H(t) dt} |\psi_k(t)\rangle. \quad (3)$$

For the classical treatment governing the lattice part of the system, on the other hand, we adopted the Euler–Lagrange equations. Their solutions can be written as a Newtonian equation able to describe the movements of the sites in the system and is given by

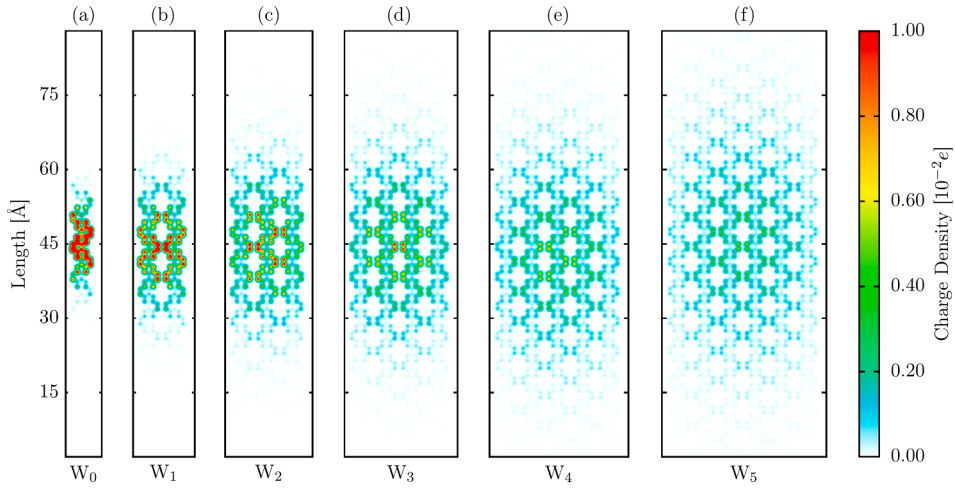


Fig. 2. Ground state solutions for the charge carrier distribution on porous nanoribbons with different widths.

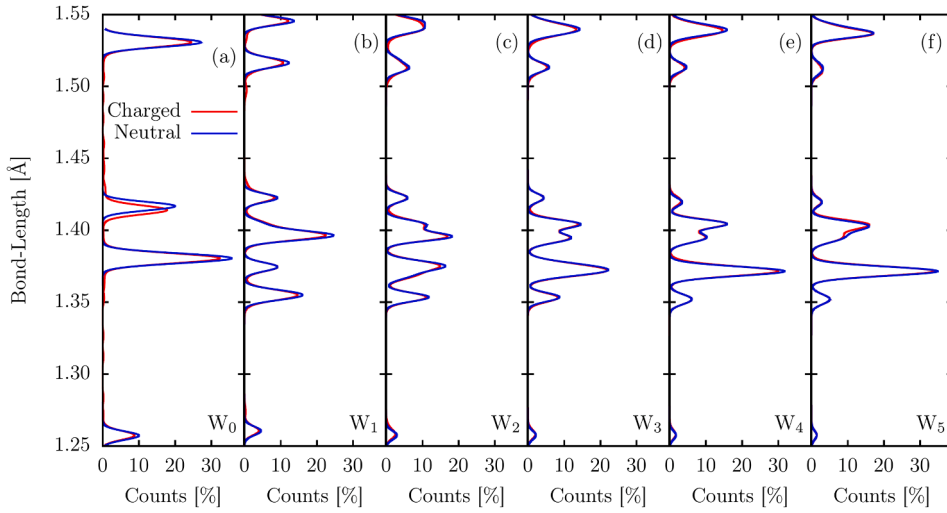


Fig. 3. Bond-length distribution along the entire length of all the neutral and charged PG nanoribbons studied here.

$$M\ddot{\eta}_{ij} = \frac{1}{2}K(\eta_{i,j'} + \eta_{i,j''} + \eta_{j,i'} + \eta_{j,i''}) - 2K\eta_{ij} + \frac{1}{2}\alpha(B_{i,j'} + B_{i,j''} + B_{j,i'} + B_{j,i''} - 4B_{ij} + \text{c.c.}), \quad (4)$$

where $B_{ij} \equiv \sum_{k,s} \psi_{k,s}^*(i,t) \psi_{k,s}(j,t)$ is the term that couples the electronic and the lattice degrees of freedom, and the prime means the summation is over occupied one-particle states.

Another crucial aspect of the model is the presence of the external electric field $\mathbf{E}(t)$. This field is included by inserting a time-dependent vector potential, $\mathbf{A}(t)$, through a Peierls Substitution for the electronic transfer integrals of the system [52], making the hopping term

$$t_{ij} = e^{-i\gamma\mathbf{A}}(t_0 - a\eta_{ij}), \quad (5)$$

where $\gamma \equiv ea/(\hbar c)$, with a being the lattice parameter ($a = 1.42$ Å in graphene nanoribbons), e being the absolute value of the electronic charge, and c the speed of light. The vector potential relates to the electric field according to $\mathbf{E}(t) = -(1/c)\dot{\mathbf{A}}(t)$. The electric field is turned on adiabatically so as to avoid artificial numerical oscillations [60]. We adopted a potential vector to introduce periodic boundary conditions for the action of the external electric field.

3. Results

We begin our discussions by characterizing the charge distribution on porous nanoribbons of different widths, as depicted in Fig. 2. For all the cases, an electron is extracted from the chain, thus obtained a net $+1e$ charged system [52]. The first feature to be noted is that as the nanoribbon gets broader, the charge is less concentrated. In Fig. 2, lattice regions with high charge concentrations are represented by the red spots. Although the overall trend is in accordance with the expected metallic behavior graphene sheets present [17,61], one can note that even for large widths the semiconducting character of the system, i.e. the carrier confinement trend, is preserved. This property can be attributed to the porosity of the system, as previous work with regular graphene nanoribbons have shown that the semiconductivity is a loss for large enough nanoribbons [27]. As a consequence, quasiparticles such as polarons tend to move substantially faster with the increase of the width [27,55]. Moreover, the charge localization is much smaller than the one previously reported in regular graphene nanoribbons of similar sizes [55,62]. These are solid indications that the nature of the charge carrier is not of a polaron, mostly for wider porous nanoribbons.

Fig. 3 shows the distribution of C–C bond-lengths for the cases presented in Fig. 2. One can note that the profiles for the charged systems are rather similar to that of the neutral ones, as can be noted in Fig. 2 (a–f). This is particularly true for broader nanoribbons. A feature that

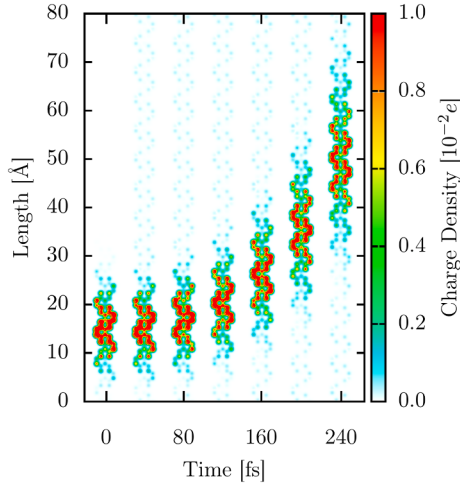


Fig. 4. Time evolution of the charge density for the system corresponding to W0 case.

can be inferred from Fig. 3(d–f) is that the bond-length configuration is not substantially altered from the width W_3 . The exception is presented in Fig. 3(a). In this case, the system resembles much more a regular graphene nanoribbon than a PG one. In broader cases, the peak around 1.37 gets larger for wider nanoribbons indicating a convergence trend for the bond-length values when the system changes from nanoribbons towards a sheet with a high surface area. Again, this trend reinforces the argument that a somewhat different scenario from that of polarons takes place in these PG nanoribbons. Differently from polaron endowed regular graphene nanoribbons, one can see in Fig. 3(b–f) that there is no substantial lattice distortions in the presence of charge when it comes to wider PG nanoribbons.

In Fig. 4 we include an external electric field of 1.0 mV/Å and simulates the charge dynamics of the W0-PG system, as a representative case. Fig. 4 presents the charge density time evolution. One can see that the charge is accelerated by the electric field, presenting a collective behavior for the excitations produced by the additional charge. This is a

definitive demonstration that the transport mechanism is mediated by polarons, as is the case in pristine armchair graphene nanoribbons [27,55]. This is so because polarons are quasiparticles defined as the collective behavior that arises from the correlation between the charge and the phonon excitations. We noted that for the transport mechanism in PG nanoribbons, even in the narrower case studied here, there is a loss of energy related to the lattice conjugation that is transferred to quasiparticle. This energy transfer process is mediated by the electron–phonon coupling term and causes the rapid acceleration of the carrier. A similar trend was reported for the transport of bipolarons in Poly(*p*-Phenylene Vinylene) lattice [63]. It is worthwhile to stress that this transport mechanism is not observed in the case of regular graphene nanoribbons [27,52,55]. The results presented in Fig. 4 suggest that polarons are responsible for mediating the charge transport mechanism in PG nanoribbons.

We conducted the same simulations for all the other widths and the same qualitative behavior is perceived, as shown in Fig. 5. The dynamics are different depending on the width of the system, as should be expected from the different structures of the initial state of Fig. 2. As a rule of thumb, the broader the nanoribbon, the larger is the charge carrier mobility. Despite the already established difference in the transport mechanism, this is a feature that is also observed in other graphene nanoribbons [62]. The polarons move in PG within the optical regime with terminal velocities varying from 0.5 up to 1.15 Å/fs, as can be inferred from Fig. 5(a–e). These velocities are lower than those for polarons in conventional graphene nanoribbons (2.2–5.1 Å/fs) [27,52,55,62]. As the electric field is turned on, the polaron moves, thus transporting the charge. In the wider cases, the polarons reach the end of the lattice very fast, thus returning to its beginning due to the periodic boundary conditions (see Fig. 5(b–e)). Since the charge movement may disturb the lattice generating phonons, the polarons encounter phonons produced by their own movement after crossing the periodic boundary conditions. This phenomenon introduced by boundary conditions choice affects the carriers producing the blurred pattern at 240 fs as presented in Fig. 5(b–e).

Finally, Fig. 6 presents the time evolution of the band structure for the charged PG nanoribbons studied here. One can note the presence of energy levels inside the bandgap (red lines). These are the levels that characterizes the polaron states. Note that as the systems get broader,

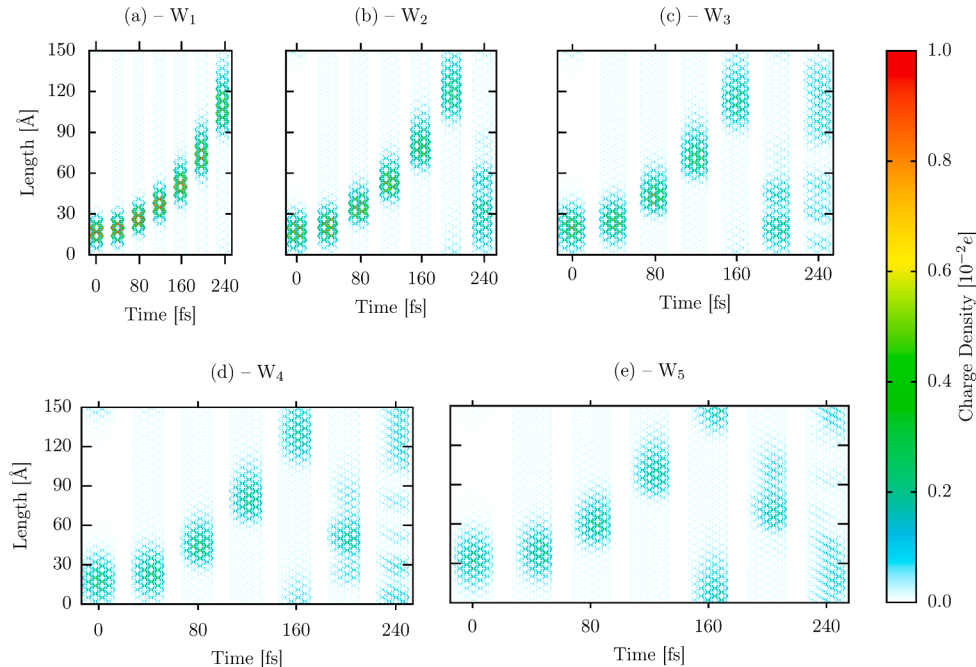


Fig. 5. Charge density time evolution of (a) W_1 , (b) W_2 , (c) W_3 , (d) W_4 , and (e) W_5 PG nanoribbons.

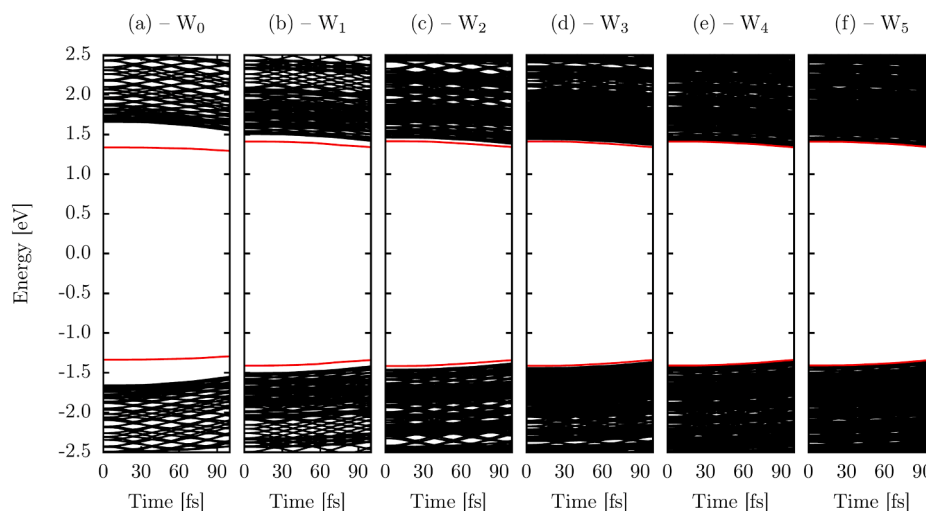


Fig. 6. Time evolution of the band structure of (a) W0, (b) W1, (c) W2, (d) W3, (e) W4, and (f) W5 PG nanoribbons.

the polaron levels approaches the conducting and valence band. As the system gets wider a more two-dimensional character prevails, thus explaining the fact that the intragap levels approach the bands. Even so, due to the width limitation of the PG nanoribbons, a semiconducting bandgap still takes place for the wider lattices.

4. Conclusions

In summary, we described polaron transport mechanism in porous graphene nanoribbons of different widths. So far, the literature had reported quasiparticles such as polarons and bipolarons to be responsible for the transport in conventional graphene nanoribbons [28,64–66]. By considering porosity, the one dimensional character that is typical of systems which exhibits such phenomena is present. It was also found that porosity works towards contributing to maintain the semiconductor nature of the nanoribbons, as we have seen that even broad nanoribbons possess a considerable finite bandgap. We noted that for the transport mechanism in PG nanoribbons, even in the narrower case studied here, there is a loss of energy related to the lattice conjugation that is transferred to the charge carrier. This process is mediated by the electron–phonon coupling term and causes the rapid acceleration of the carrier. Importantly, this transport mechanism is not observed in the case of regular graphene nanoribbons [27,52,55]. In PG nanoribbons, the charge is accelerated by the electric field and there is no corresponding distortion following the center of charge. These results suggest that polarons are responsible for mediating the charge transport mechanism in PG nanoribbons. As a rule, the broader the nanoribbon, the larger is the charge carrier mobility. The polarons move in PG within the optical regime with terminal velocities varying from 0.5 Å/fs up to 1.15 Å/fs. These velocities are lower than the ones for polarons in regular graphene nanoribbons (2.2–5.1 Å/fs) [27,55,62].

CRediT authorship contribution statement

Wiliam F. da Cunha: Data curation, Formal analysis, Methodology, Writing - original draft. **Marcelo L. Pereira Júnior:** Data curation, Formal analysis, Methodology, Writing - original draft. **William F. Giazza:** Data curation, Formal analysis, Methodology, Writing - original draft. **Rafael T. de Sousa Junior:** Conceptualization, Supervision, Funding acquisition, Writing - review & editing. **Luiz A. Ribeiro Júnior:** Conceptualization, Supervision, Funding acquisition, Writing - review & editing. **Geraldo M. e Silva:** Conceptualization, Supervision, Funding acquisition, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

The authors gratefully acknowledge the financial support from Brazilian Research Councils CNPq, CAPES, and FAPDF and CENAPAD-SP for providing the computational facilities. M.L.P.J. gratefully acknowledge the financial support from CAPES grant 88882.383674/2019-01. L. A.R.J. and W.F.G. gratefully acknowledge the financial support from FAP-DF grant 0193.0000248/2019-32. L.A.R.J. and G.M.S gratefully acknowledge, respectively, the financial support from CNPq grants 302236/2018-0 and 304637/2018-1. R.T.S.J. gratefully acknowledge, respectively, the financial support from CNPq grants 465741/2014-2 and 312180/2019-5, CAPES grant 88887.144009/2017-00, and FAP-DF grants 0193.001366/2016 and 0193.001365/2016. L.A.R.J. gratefully acknowledges the financial support from DPI/DIRPE/UnB (Edital DPI/DPG 03/2020) grant 23106.057541/2020-89 and from IFD/UnB (Edital 01/2020) grant 23106.090790/2020-86.

References

- [1] P. Yang, J.M. Tarascon, Towards systems materials engineering, *Nature Materials* 11 (7) (2012) 560–563.
- [2] J. Allison, D. Backman, L. Christodoulou, Integrated computational materials engineering: a new paradigm for the global materials profession, *Jom* 58 (11) (2006) 25–27.
- [3] J.A. Hubbell, S.N. Thomas, M.A. Swartz, Materials engineering for immunomodulation, *Nature* 462 (7272) (2009) 449–460.
- [4] S.J. Simske, R.A. Ayers, T.A. Bateman, Porous materials for bone engineering, in: *Materials Science Forum*, Trans Tech Publ, 1997, vol. 250, pp. 151–182.
- [5] A.K. Geim, K.S. Novoselov, The rise of graphene, in: *Nanoscience and Technology: A Collection of Reviews from Nature Journals*, World Scientific, 2010, pp. 11–19.
- [6] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I. V. Grigorieva, A.A. Firsov, Electric field effect in atomically thin carbon films, *Science* 306 (5696) (2004) 666–669.
- [7] K.S. Novoselov, Nobel lecture: graphene: materials in the flatland, *Reviews of Modern Physics* 83 (3) (2011) 837.
- [8] K.S. Novoselov, S.V. Morozov, T.M.G. Mohinddin, L.A. Ponomarenko, D.C. Elias, R. Yang, I.I. Barbolina, P. Blake, T.J. Booth, D. Jiang, J. Giesbers, A.K. Geim, Electronic properties of graphene, *Physica Status Solidi (b)* 244 (11) (2007) 4106–4111.
- [9] A.H.C. Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, A.K. Geim, The electronic properties of graphene, *Reviews of Modern Physics* 81 (1) (2009) 109.
- [10] J. Kotakoski, C. Mangler, J.C. Meyer, Imaging atomic-level random walk of a point defect in graphene, *Nature Communications* 5 (1) (2014) 1–5.

- [11] R.A. Soler-Crespo, W. Gao, P. Xiao, X. Wei, J.T. Paci, G. Henkelman, H.D. Espinosa, Engineering the mechanical properties of monolayer graphene oxide at the atomic level, *The Journal of Physical Chemistry Letters* 7 (14) (2016) 2702–2707.
- [12] J. Lahiri, Y. Lin, P. Bozkurt, I.I. Oleynik, M. Batzill, An extended defect in graphene as a metallic wire, *Nature Nanotechnology* 5 (5) (2010) 326.
- [13] A.W. Robertson, C.S. Allen, Y.A. Wu, K. He, J. Olivier, J. Neethling, A.I. Kirkland, J. H. Warner, Spatial control of defect creation in graphene at the nanoscale, *Nature Communications* 3 (1) (2012) 1–7.
- [14] A.C. Ferrari, F. Bonaccorso, V. Fal'Ko, K.S. Novoselov, S. Roche, P. Bøggild, S. Borini, F.H.L. Koppens, V. Palermo, N. Pugno, et al., Science and technology roadmap for graphene, related two-dimensional crystals, and hybrid systems, *Nanoscale* 7 (11) (2015) 4598–4810.
- [15] Q. Tang, Z. Zhou, Z. Chen, Graphene-related nanomaterials: tuning properties by functionalization, *Nanoscale* 5 (11) (2013) 4541–4583.
- [16] F. Bonaccorso, L. Colombo, G. Yu, M. Stoller, V. Tozzini, A.C. Ferrari, R.S. Ruoff, V. Pellegrini, Graphene, related two-dimensional crystals, and hybrid systems for energy conversion and storage, *Science* 347 (6217) (2015).
- [17] V. Singh, D. Joung, L. Zhai, S. Das, S.I. Khondaker, S. Seal, Graphene based materials: past, present and future, *Progress in Materials Science* 56 (8) (2011) 1178–1271.
- [18] D. Li, R.B. Kaner, Graphene-based materials, *Nature Nanotechnology* 3 (2008) 101.
- [19] X. Huang, Z. Yin, S. Wu, X. Qi, Q. He, Q. Zhang, Q. Yan, F. Boey, H. Zhang, Graphene-based materials: synthesis, characterization, properties, and applications, *Small* 7 (14) (2011) 1876–1902.
- [20] M. Bieri, M. Treier, J. Cai, K. Ait-Mansour, P. Ruffieux, O. Gröning, P. Gröning, M. Kastler, R. Rieger, X. Feng, K. Müllen, R. Fasel, Porous graphenes: two-dimensional polymer synthesis with atomic precision, *Chemical Communications* 1 (45) (2009) 6919–6921.
- [21] L. Jiang, Z. Fan, Design of advanced porous graphene materials: from graphene nanomesh to 3d architectures, *Nanoscale* 6 (4) (2014) 1922–1945.
- [22] M. Hatanaka, Band structures of porous graphenes, *Chemical Physics Letters* 488 (4–6) (2010) 187–192.
- [23] D. Jiang, V.R. Cooper, S. Dai, Porous graphene as the ultimate membrane for gas separation, *Nano Letters* 9 (12) (2009) 4019–4024.
- [24] J. Yan, Z. Fan, W. Sun, G. Ning, T. Wei, Q. Zhang, R. Zhang, L. Zhi, F. Wei, Advanced asymmetric supercapacitors based on ni (oh) 2/graphene and porous graphene electrodes with high energy density, *Advanced Functional Materials* 22 (12) (2012) 2632–2641.
- [25] K. Celebi, J. Buchheim, R.M. Wyss, A. Droudian, P. Gasser, I. Shorubalko, J. Kye, C. Lee, H.G. Park, Ultimate permeation across atomically thin porous graphene, *Science* 344 (6181) (2014) 289–292.
- [26] S.P. Koenig, L. Wang, J. Pellegrino, J.S. Bunch, Selective molecular sieving through porous graphene, *Nature Nanotechnology* 7 (11) (2012) 728–732.
- [27] W.F. da Cunha, P.H. Acioli, P.H. de Oliveira Neto, R. Gargano, G.M. e Silva, Polaron properties in armchair graphene nanoribbons, *The Journal of Physical Chemistry A* 120 (27) (2016) 4893–4900.
- [28] G.G. Silva, L.A. Ribeiro Junior, M.L. Pereira Junior, A.L.A. Fonseca, R.T. Sousa Júnior, Geraldo m. e. silva, bipolaron dynamics in graphene nanoribbons, *Scientific Reports* 9 (2019) 2909.
- [29] A.V.P. Abreu, L.A. Ribeiro Junior, G.G. Silva, M.L. Pereira Junior, B.G. Enders, A.L. A. Fonseca, G.M. e Silva, Stability conditions of armchair graphene nanoribbon bipolarons, *Journal of Molecular Modeling* 25 (8) (2019) 245.
- [30] J. Cai, P. Ruffieux, R. Jaafar, M. Bieri, T. Braun, S. Blankenburg, M. Muoth, A. P. Seitsonen, M. Saleh, X. Feng, et al., Atomically precise bottom-up fabrication of graphene nanoribbons, *Nature* 466 (7305) (2010) 470–473.
- [31] Y. Son, M.L. Cohen, S.G. Louie, Energy gaps in graphene nanoribbons, *Physical Review Letters* 97 (21) (2006), 216803.
- [32] Y. Son, M.L. Cohen, S.G. Louie, Half-metallic graphene nanoribbons, *Nature* 444 (7117) (2006) 347–349.
- [33] M.Y. Han, B. Özyilmaz, Y. Zhang, P. Kim, Energy band-gap engineering of graphene nanoribbons, *Physical Review Letters* 98 (20) (2007), 206805.
- [34] M.Y. Han, J.C. Brant, P. Kim, Electron transport in disordered graphene nanoribbons, *Physical Review Letters* 104 (5) (2010), 056801.
- [35] K. Wakabayashi, Y. Takane, M. Yamamoto, M. Sgrist, Electronic transport properties of graphene nanoribbons, *New Journal of Physics* 11 (9) (2009), 095016.
- [36] F.J. Martín-Martínez, S. Fias, G. Van Lier, F. De Proft, P. Geerlings, Electronic structure and aromaticity of graphene nanoribbons, *Chemistry—A European Journal* 18 (20) (2012) 6183–6194.
- [37] J. Baringhaus, M. Ruan, F. Edler, A. Tejada, M. Sicot, A. Taleb-Ibrahimi, A. Li, Z. Jiang, E.H. Conrad, C. Berger, et al., Exceptional ballistic transport in epitaxial graphene nanoribbons, *Nature* 506 (7488) (2014) 349–354.
- [38] Z. Li, H. Qian, J. Wu, B. Gu, W. Duan, Role of symmetry in the transport properties of graphene nanoribbons under bias, *Physical Review Letters* 100 (20) (2008), 206802.
- [39] M.L. Pereira Júnior, L.A. Ribeiro Júnior, Thermomechanical insight into the stability of nanoporous graphene membranes, *FlatChem* 24 (2020), 100196.
- [40] J. Xiao, D. Mei, X. Li, W. Xu, D. Wang, G.L. Graff, W.D. Bennett, Z. Nie, L.V. Saraf, I. A. Aksay, et al., Hierarchically porous graphene as a lithium–air battery electrode, *Nano Letters* 11 (11) (2011) 5071–5078.
- [41] Y. Tao, Q. Xue, Z. Liu, M. Shan, C. Ling, T. Wu, X. Li, Tunable hydrogen separation in porous graphene membrane: first-principle and molecular dynamic simulation, *ACS Applied Materials & Interfaces* 6 (11) (2014) 8048–8058.
- [42] M. Hankel, Y. Jiao, A. Du, S.K. Gray, S.C. Smith, Asymmetrically decorated, doped porous graphene as an effective membrane for hydrogen isotope separation, *The Journal of Physical Chemistry C* 116 (11) (2012) 6672–6676.
- [43] P. Xu, J. Yang, K. Wang, Z. Zhou, P. Shen, Porous graphene: properties, preparation, and potential applications, *Chinese Science Bulletin* 57 (23) (2012) 2948–2955.
- [44] R. Mukherjee, A.V. Thomas, D. Datta, E. Singh, J. Li, O. Eksik, V.B. Shenoy, N. Koratkar, Defect-induced plating of lithium metal within porous graphene networks, *Nature Communications* 5 (1) (2014) 1–10.
- [45] G. Brunetto, P.A.S. Autreto, L.D. Machado, B.I. Santos, R.P.B. Santos, D.S. Galvao, Nonzero gap two-dimensional carbon allotrope from porous graphene, *The Journal of Physical Chemistry C* 116 (23) (2012) 12810–12813.
- [46] S.K. Singh, D. Kumar, V.M. Dhavale, S. Pal, S. Kurungot, Strategic preparation of efficient and durable nico alloy supported n-doped porous graphene as an oxygen evolution electrocatalyst: A theoretical and experimental investigation, *Advanced Materials Interfaces* 3 (20) (2016) 1600532.
- [47] Y. Lu, H. Lyu, A.G. Richardson, T.H. Lucas, D. Kuzum, Flexible neural electrode array based-on porous graphene for cortical microstimulation and sensing, *Scientific Reports* 6 (2016) 33526.
- [48] S.P. Surwade, S.N. Smirnov, I.V. Vlassiuk, R.R. Unocic, G.M. Veith, S. Dai, S. M. Mahurin, Water desalination using nanoporous single-layer graphene, *Nature Nanotechnology* 10 (5) (2015) 459–464.
- [49] A. Du, Z. Zhu, S.C. Smith, Multifunctional porous graphene for nanoelectronics and hydrogen storage: new properties revealed by first principle calculations, *Journal of the American Chemical Society* 132 (9) (2010) 2876–2877.
- [50] J. Schrier, Helium separation using porous graphene membranes, *The Journal of Physical Chemistry Letters* 1 (15) (2010) 2284–2287.
- [51] G.M. e Silva, Electric field effects o the competition between polarons and bipolarons in conjugated polymers, *Physical Review B* 61 (2000) 10777.
- [52] W.F. Cunha, P.H. Oliveira Neto, L.A. Ribeiro Junior, G.M. e Silva, Quasiparticle description of transition metal dichalcogenide nanoribbons, *Physical Review B* 99 (3) (2019), 035405.
- [53] V. Barone, O. Hod, G.E. Scuseria, Electronic structure and stability of semiconducting graphene nanoribbons, *Nano Letters* 6 (12) (2006) 2748–2754.
- [54] P.H. de Oliveira Neto, J.F. Teixeira, W.F. da Cunha, R. Gargano, G.M. e Silva, Electron–lattice coupling in armchair graphene nanoribbons, *The Journal of Physical Chemistry Letters* 3 (20) (2012) 3039–3042.
- [55] L.A. Ribeiro Jr, W.F. da Cunha, A.L. de Almeida Fonseca, G.M. e Silva, S. Stafström, Transport of polarons in graphene nanoribbons, *The Journal of Physical Chemistry Letters* 6 (3) (2015) 510–514.
- [56] V.N. Kotov, B. Uchoa, V.M. Pereira, F. Guinea, A.H.C. Neto, Electron-electron interactions in graphene: current status and perspectives, *Reviews of Modern Physics* 84 (3) (2012) 1067.
- [57] J. Yan, Y. Zhang, P. Kim, A. Pinczuk, Electric field effect tuning of electron-phonon coupling in graphene, *Physical Review Letters* 98 (16) (2007), 166802.
- [58] A.H.C. Neto, N.M.R. Peres, K.S. Novoselov, A.K. Geim, The electronic properties of graphene, *Review Modern Physics* 81 (109) (2009) 1–55.
- [59] J. Yan, Y. Zhang, S. Goler, P. Kim, A. Pinczuk, Raman scattering and tunable electron–phonon coupling in single layer graphene, *Solid State Communications* 143 (1–2) (2007) 39–43.
- [60] L.A. Ribeiro Jr, W.F. da Cunha, P.H. de Oliveira Neto, R. Gargano, G.M. e Silva, Impurity effects on polaron-exciton formation in conjugated polymers, *The Journal of Chemical Physics* 139 (17) (2013), 174903.
- [61] J.C. Garcia, D.B. de Lima, L.V.C. Assali, J.F. Justo, Group iv graphene-and graphene-like nanosheets, *The Journal of Physical Chemistry C* 115 (27) (2011) 13242–13246.
- [62] G.G. Silva, W.F. da Cunha, R.T. Sousa Junior, A.L.A. Fonseca, L.A. Ribeiro Júnior, G.M. e Silva, Influence of quasi-particle density over polaron mobility in armchair graphene nanoribbons, *Physical Chemistry Chemical Physics* 20 (24) (2018) 16712–16718.
- [63] Fábio Luís de Oliveira Paula, Leonardo Luiz e Castro, Luiz Antonio Ribeiro Junior, Rafael Timóteo de Sousa Júnior, Geraldo Magela e Silva, Pedro Henrique de Oliveira Neto, Dynamical mechanism of polarons and bipolarons in poly (p-phenylene vinylene), *Scientific Reports* 9 (1) (2019) 1–7.
- [64] M.L. Pereira Junior, W.F. da Cunha, R.T. Sousa Júnior, W.F. Giazza, G.M. e Silva, L. A. Ribeiro Junior, Charge transport mechanism in chevron-graphene nanoribbons, *The Journal of Physical Chemistry C* (2020).
- [65] M.L. Pereira Junior, P.H. Oliveira Neto, L.E. Sousa, L.A. Ribeiro Junior, et al. Charge localization and hopping in a topologically engineered gnr, *arXiv preprint arXiv:2007.10913*, 2020.
- [66] M.L. Pereira Júnior, B.G. Enders Neto, W.F. Giazza, R.T. de Sousa Junior, G.M. e Silva, L.A. Ribeiro Junior, Transport of quasiparticles in coronene-based graphene nanoribbons, *Journal of Materials Chemistry C* (2020).