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## RESEARCH ARTICLE

# Current-Voltage Characterization of Multi-Port Graphene Based Geometric Diodes for High-Frequency Electromagnetic Harvesting

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**ABSTRACT** In this contribution, geometric diodes based on graphene patterned with spatial asymmetry have been studied, starting from tight-binding numerical approximation in a self-consistent framework, to verify their potential for electromagnetic (e. m.) harvesting. We report a detailed analysis of coherent charge transport and provide some figures of merit with respect to e. m. rectification, such as, for instance, the asymmetry of the dark current-voltage characteristics. The most important achievement of this work is given by the accurate analysis of the main key physical/geometric parameters that affect the nonlinear response of the diodes, for different configurations and geometries. Owing to the Scattering Matrix approach, introduced elsewhere for coherent transport calculation, it was possible to cascade asymmetric discontinuities and simulate large structures (more than 100K atoms) in a modular fashion. In this way, simulation at the atomistic level can be brought up to the device level to provide guidelines for design and fabrication, in view of practical applications related to clean-energy harvesting/rectification up to infrared and solar-light frequencies.

**INDEX TERMS** Geometric diode, quantum transport, electromagnetic harvesting.

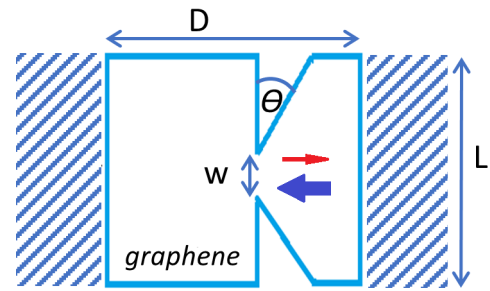
## I. INTRODUCTION

One of the main challenges in developing geometric diodes for THz to optical harvesting [1], [2], [3], [4], [5], [6], [7], [8], [9], [10], [11], [12], [13], [14], [15] resides in a mean-free-path (MFP) higher than the critical dimensions of the diode, in such a way that charge wavefunctions can be properly affected by the geometrical asymmetry. For that reason, graphene, which has a relatively large MFP, was tentatively used as conducting layer in these diodes, as described in [2], where the I-V characteristics can be tuned and even reversed by applying a gate field. In rectennas, these devices have been demonstrated at 28 THz. The concept of geometric diodes is closely related to the ballistic regime of charge transport. The diode-like response is seen, in this case, as a

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collective (continuous) motion of particle systems in a well-defined direction, upon excitation from an external source of energy and momentum, such as an electromagnetic impinging wave having zero temporal/spatial average (sinusoidal signal). Such effect is sustained without violating the second law of Thermodynamics, owing to the topological asymmetry (or time reversal perturbation) experienced by charge carriers during their propagation. In that respect, it is evident the analogy with photovoltaic effect, based on the asymmetry at a microscopic level resulting from spatially varying electronic band structure. An interesting example of asymmetry-driven transport is given by the “ratchet effect”, originally introduced by Feynman in 1963 [16]. Several devices try to implement the ratchet concept [17], [18], [19], [20], [21], [22], [23], [24]: nano-patterns of asymmetric dots in two-dimensional electron gas (2DEG) at surface heterostructures and biological molecular motors, where the Brownian random molecular

motion (thermal fluctuation) gives rise to specific - linear of rotational - movements. One of the potential advantages of ballistic planar diodes with respect to other configurations, such as MIMs, is given by their typically small capacitive effects, in contrast to the relatively high capacitance of MIM diodes, where two parallel metal plates are overlapping at short distance. In addition, the diode resistivity could be, in principle, sufficiently low (non-tunneling current) to allow good matching with the input impedance of metallic antennas. For the typical size of diodes considered in this work (few hundreds  $nm^2$  of graphene area), the geometric capacitance is in the range of  $aF$ , which provides RC time constants in the range of  $fs$ , i. e. lower than, or comparable with, the time-period of the visible light. In order to describe ballistic transport at nanoscale, simulations are performed in the framework of the Scattering Matrix (SM) approach, described elsewhere [25], [26], which constitutes a formulation of the Landauer-Büttiker method equivalent to the non-equilibrium Green's function formalism (NEGF). In fact, SM is able to provide non only transmission/reflection coefficients but also the Green's function in absence of anelastic scattering between charges and phonon modes. Differently from continuous transport models, like the ones based on Dirac or Kubo approximations [27], [28], the above model allows atomistic description, although approximated, of abrupt discontinuities and spatial asymmetries, taking also into account chirality and edge conditions that could be important at nanoscale. Abrupt discontinuities also imply scattering between the two Dirac points of graphene and makes a single "valley" picture potentially not reliable. In addition, the Dirac approach also assumes the approximation of linear bands of single layer graphene. To capture effects of the atomic structure, including the influence of defect boundaries, and to provide a realistic description of the band structure including band bending at high energies, we need to go beyond the Dirac fermion model. An important feature of SM approach is the possibility to cascade or combine different sub-modules, connecting the S-matrices of different sub-parts of the entire computational domain. Moreover, the SM approach has the advantage, over other methods like DFT/ab-initio techniques, that a full-wave analysis can be carried out for very large structures ( $>100K$  atoms), accounting for the real wave nature of charges and multimodality of transport. Monte-Carlo methods could hardly calculate the interference/tunneling/scattering effects related to the wave nature of electronic channels, whose wavelength is comparable with, or larger than, the asymmetry. On the other hand, SM describes of charge transport in terms of propagating and evanescent modes, much like the standard analysis of periodically loaded microwave waveguides in terms of circuit ports. Electronic channels are treated as propagating or evanescent modes coupled by lattice discontinuities and potential variations, making possible a clear evaluation of how different charges interact and contribute to the physical current through the graphene lattice. Depending on the applied voltage and on the size of the graphene structure considered, we compute the effect of up



**FIGURE 1. Graphene-based geometric diode. Red and blue arrows suggests the imbalance of charge flow due to the geometric asymmetry.**

to  $K > 100$  electronic channels simultaneously for any of the  $N$  physical ports that define the inputs/outputs, resulting in typical scattering matrices of size  $[k \cdot N, k \cdot N]$ . We start with  $N = 2$  (two port graphene circuit) both for single and cascaded asymmetries, and finally consider the case of  $N = 3$  (three port Y-shaped graphene circuit).

## II. THEORY AND PROBLEM STATEMENT

In some respects, graphene technology is in its infancy, and the standard nanofabrication processes and chemicals that are used successfully to fabricate structures from other materials can degrade the electronic quality of graphene. In addition, graphene geometric diodes still need effort to engineer and improve their nonlinear response for efficient high frequency rectennas. In the present work, a linear taper in graphene is assumed as a starting simplified geometry for numerical simulation, with reference to Fig. 1. The orientation of carbon lattice and graphene edge, with respect to the external applied field and to charge propagation direction, is taken into account differently from what is done in continuum models. Owing to their long mean free path, charges scattered through the asymmetric taper are likely to reach the other side before the occurrence of other scattering events, like collisions with other carriers or impurities. Thus, charges are collected to the metal contacts, giving rise to a current flow. The spatial asymmetry of the defect pattern, in combination with an external forcing electromagnetic field, implies a preferred direction for the charge flow, namely in the direction of decreasing graphene width. The same design principle was used for creation of detectors operating at room temperature in the microwave/terahertz radiation range [1]. As widely reported in the literature, the test-bed case of Fig. 1 allows a numerical check on how a simple spatial symmetry can affect the asymmetry of charge transport.

The main technical objective of the following quantum-transport analysis is to provide the dependence of current-voltage curves on geometric and physical parameters. In particular, with reference to Fig. 1:

- 1) the size of the graphene area  $D \cdot L$ ,
- 2) the angle  $\theta$  formed by the boundaries of the graphene neck,
- 3) the neck width  $w$ ,

4) the initial charge density  $n$  of the graphene layer that is used for subsequent patterning.

The latter can be easily calculated according to its nominal Fermi level  $E_F$ :

$$n = \int f(E, E_F) \frac{2E}{\pi(h_t v_F)^2} dE \quad (1)$$

where  $h_t$  is the Plank constant,  $f$  is the Fermi statistic, and  $v_F$  is the Fermi velocity. The final goal of the modelling is to find an optimum configuration of parameters 1-4 in terms of the following criteria:

- asymmetry of the I-V characteristic, as high as possible,
- diode resistance, related to the forward-bias current, possibly so low as to be compatible with the impedance with the EM-field receiving system,
- reverse-bias current, ideally zero.

Considering a graphene circuit with  $N$  physical ports, the TB Hamiltonian  $H$  [9] is updated by self-generated potential due to charge propagation, after numerical convergence of the Poisson-Schrödinger system of equations. In a first approximation,  $H$  could be directly used for current estimation. The latter is calculated, in general, summing up all contributions to the charge transmittivity ( $T$ ) among all the ports. For instance, the current carried by the  $q$ -th mode of the  $m$ -th port is given by transmittivity contributions from every mode ( $p$  index of summation) propagating at all the other ports ( $n$  index of summation):

$$I_m^q = \frac{2e^2}{h} \int \left[ \sum_{n=1, n \neq m}^N \sum_p T_{m,n}^{p,q}(E) \right] dE \quad (2)$$

Fermi probability is omitted for better readability. The total current at the generic  $m$ -th port follows as:

$$I_m = \sum_q I_m^q \quad (3)$$

Other possible geometric asymmetries could be compared to the chosen one, in terms of above criteria. Clearly, satisfying one or two of these could not be beneficial for rectification if the others are not properly met. Numerical results are consistent with those of [1], where the currents are in the range of fractions of mA and the voltage dependence show relatively low asymmetry.

### III. NUMERICAL RESULTS AND DISCUSSION

#### A. ANALYSIS OF PARAMETER SENSITIVITY

As a first test, we evaluate the effect of the size of the graphene diode - or the diode area - while keeping same aperture/neck size. It is evident from Fig. 2 that, decreasing such size, the I-V asymmetry increases, and both forward and reverse current reduce (diode impedance increases). In the inset, the asymmetry ( $Asym$ ) is evaluate as  $I(V)/I(-V)$ : to avoid interpolations and numerical artifacts, the curves are plotted using a limited amount of calculated points - due to their high computational cost - so that variations are not

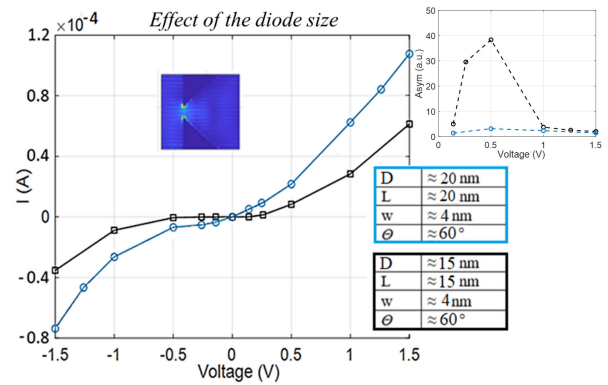


FIGURE 2. I-V for two diodes with same value of  $w$ : blue and black curves are obtained with  $L = D = 20$  nm and  $L = D = 15$  nm respectively.

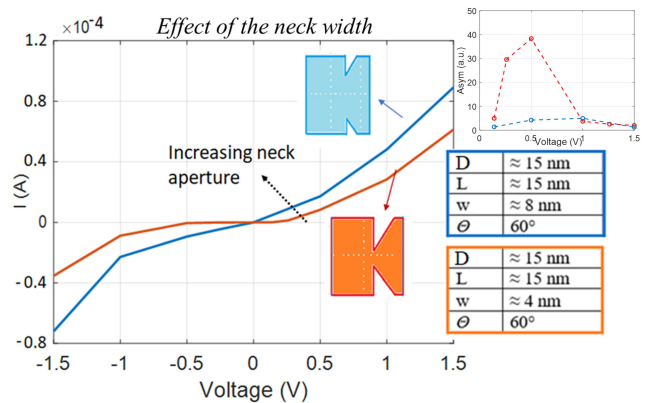


FIGURE 3. I-V obtained with  $w = 4$  nm (orange) and  $w = 8$  nm (blue), with  $D = L = 15$  nm.

smooth but can still provide quantitative information about the related numbers.

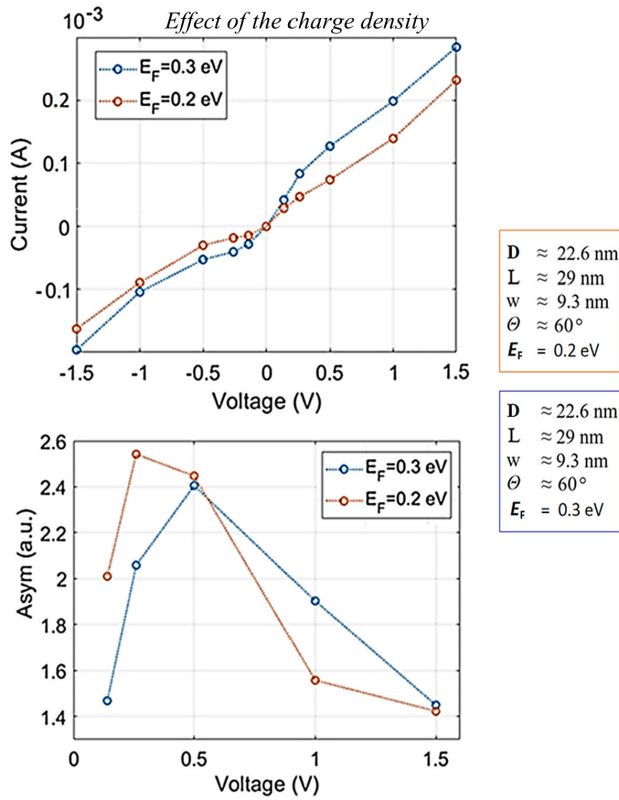
To evaluate the effect of the neck width  $w$ , we keep now fixed the diode area. From Fig. 3, we can observe that decreasing  $w$ : the I-V asymmetry increases, and both forward and reverse (absolute value) currents reduce.

The next parameter to be considered is the charge density  $n$ : Fig. 4 shows that, decreasing  $n$ , the I-V asymmetry slightly increases and shifts to lower voltages, and both forward and reverse (absolute value) currents reduce (Fig. 4(b)).

Finally, in Fig. 5, let have a look to the effect of the angle  $\theta$  on I-V curves. Decreasing  $\theta$  we observe that:

- the I-V asymmetry decreases,
- the forward current decreases and the reverse current (absolute value) increases.

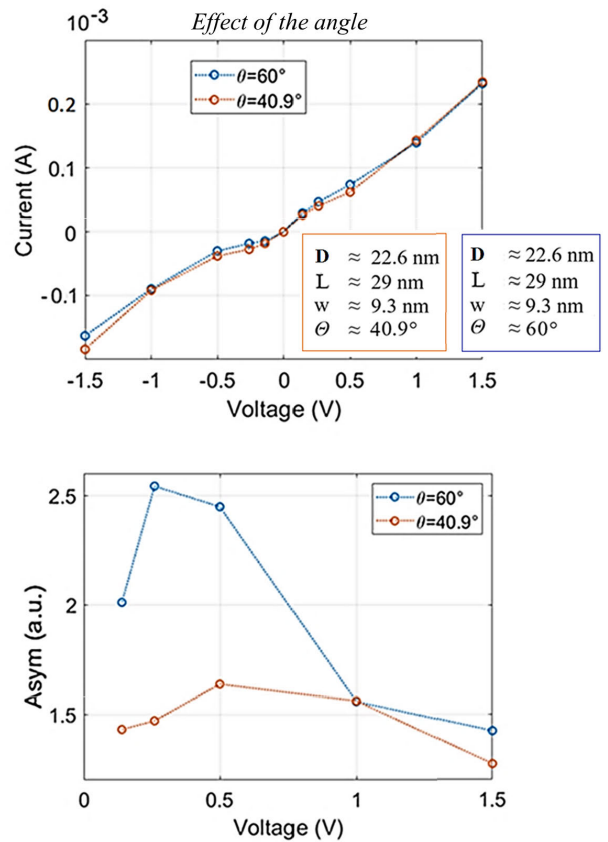
It is worth to comment a bit more about the sensitivity of the I-V curves to  $\theta$ . It may seem that increasing the latter produce only benefits because the asymmetry increases and the impedance reduces, together with a reverse current closer to zero. As a matter of fact, such good trend saturates already at about 60°: increasing  $\theta$  to 70° does not produce further benefits in terms of asymmetry or impedance.



**FIGURE 4.** Top picture shows the I-V curves for diodes with same geometry (see insets) but different charge density:  $E_F = 0.2$  eV and  $E_F = 0.3$  eV for orange and blue curves respectively; the bottom picture compares the asymmetry calculated for the above two diodes.

**B. ADDITIONAL CONSIDERATIONS**

A typical figure of merit related to the above I-V curves is given by the responsivity. This is a key parameter for rectification efficiency and potentially for e.m. harvesting [29]. The current responsivity is related to the second derivative of the current with respect to the voltage normalized to the first derivative, namely  $Resp = I''(V)/I'(V)$ . The latter can be viewed as the DC current generated per unit AC power incident on the diode. In addition, we report the nonlinearity, defined as  $\chi = I'(V)/(I/V)$ . All the above results, for the case  $L = 15$  nm,  $D = 15$  nm,  $w = 4$  nm, are reported in Fig. 6. It can be observed that, as the voltage departs from the origin, the quality of diode response rapidly decays in terms of the above figures of merit, after an initial maximum at a small fraction of V. This general trend is due basically to the high number of electronic channels involved in charge transport at high energies, whose contribution to the current mitigate the effect of the geometric asymmetry (small ripples are less significant as just related to the numerical fitting of the simulated data). Such a behavior is significantly different from that of graphene-MIM diodes [30] where maxima of asymmetry of responsivity occur at relatively higher voltages. This property may suggest that a hybrid solution for the diode, i.e. graphene MIM and geometric asymmetric, could help covering a wider range of voltages.

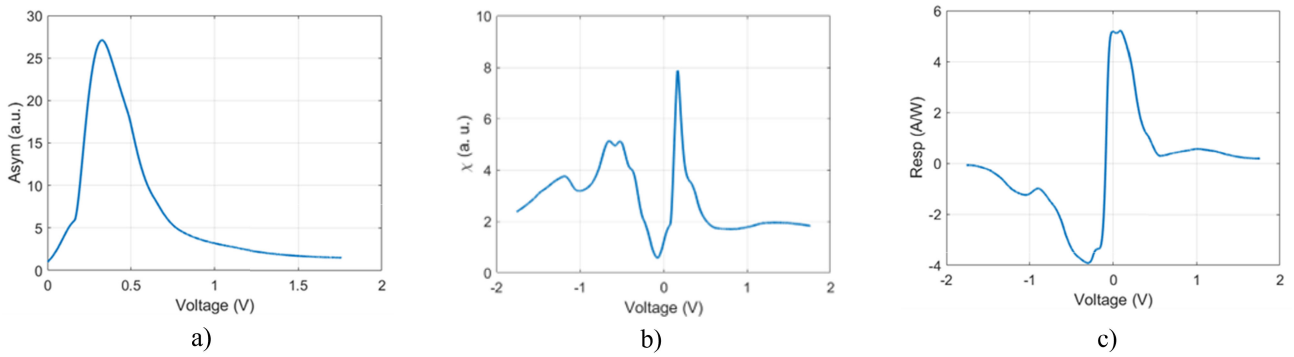


**FIGURE 5.** The top part of the figure shows the I-V curves for diodes with different value for the angle, namely  $\theta = 60^\circ$  and  $\theta = 40.9^\circ$  for blue and orange curves respectively; the bottom picture compares the asymmetry calculated for the above two diodes.

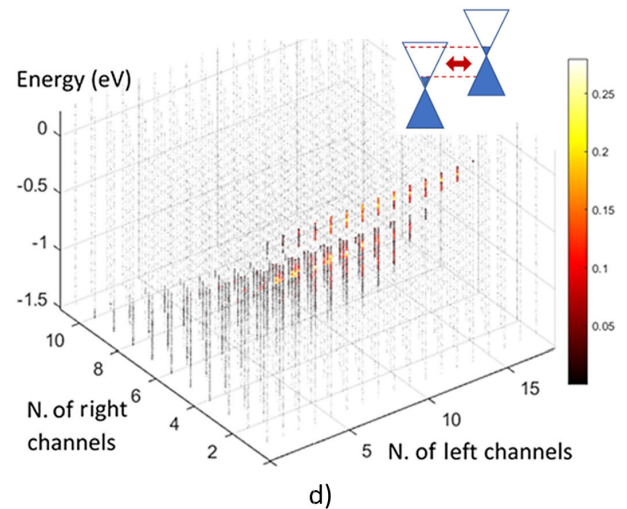
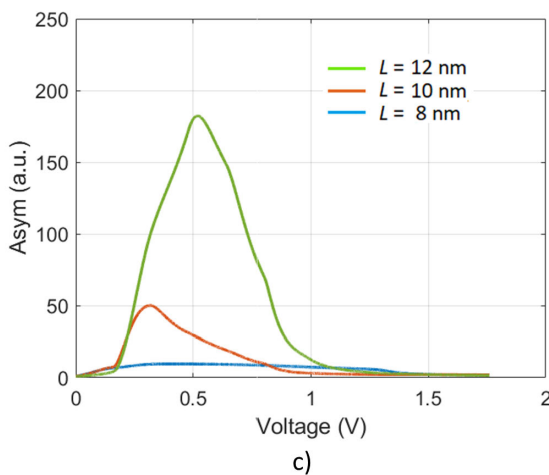
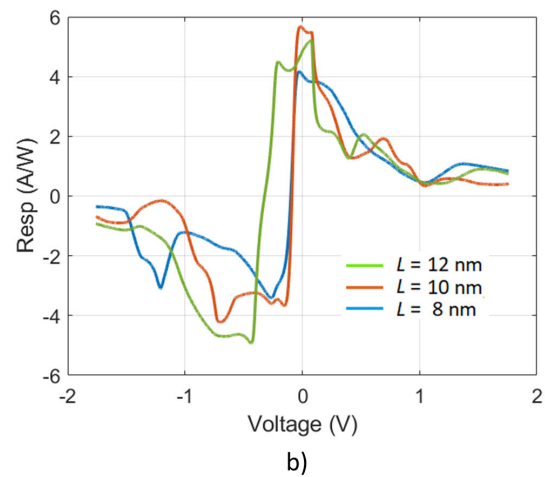
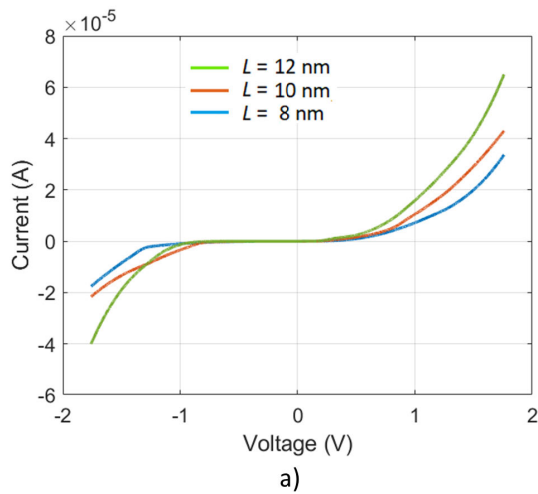
It is also interesting to push the diode geometry down to the physical limit - although not practically feasible - of  $w = 1$  nm. The objective is to provide an estimation of the figures of merit of the above diodes in the limit case of very small size, and completely ideal conditions (transparent metal contacts, no Fermi-level or wave-function mismatch with metals). Figure 7 reports the figures of merits, obtained in different cases: extremely small graphene diodes where  $L = [8$  nm, 10 nm, 12 nm],  $D = 15$  nm, and the triangular-shape restriction with  $w = 1$  nm. In these hypothetical cases the I-V curves would get much more asymmetric, but at the price of very small amounts of current and of higher diode impedences.

For completeness, Fig. 7d reports an example of charge transmittivity  $T$  across the graphene diode, for a voltage difference of 1.76 V. Fixed the external voltage, charge direction is not relevant for the transmittivity, owing to reciprocity. However, when a voltage with opposite sign is considered, the transmittivity changes due to the superposition between voltage and asymmetric geometry, so that I-V asymmetry follows. The latter is calculated by summing the net transmittivity over all energies, as indicated in Eq. 2, 3, weighted by the Fermi function at a given temperature.





**FIGURE 6.** Simulated curves after fitting of the raw output data, for the diode with  $L = 15$  nm,  $D = 15$  nm,  $w = 4$  nm,  $\theta = 60^\circ$ ,  $E_F = 0.2$  eV. a) Asymmetry, b) Nonlinearity, c) Responsivity.

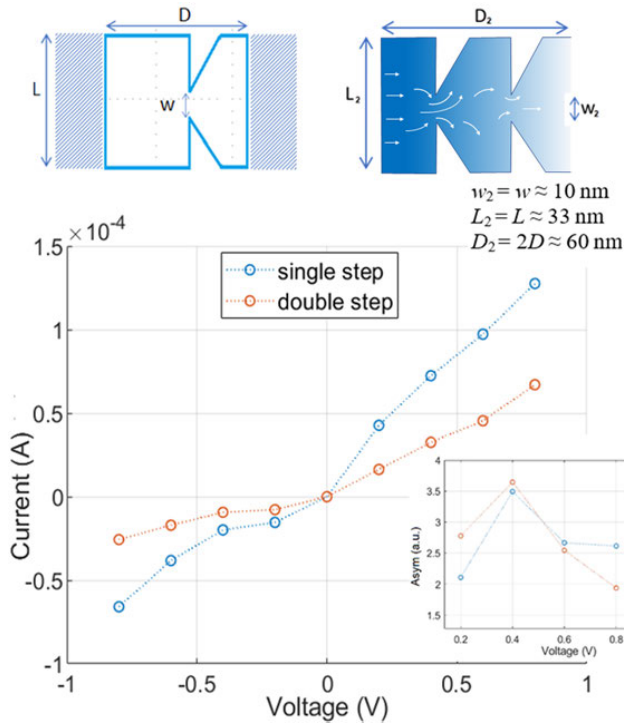


**FIGURE 7.** Results for graphene diodes with  $w = 1$  nm and  $L = [8$  nm,  $10$  nm,  $12$  nm],  $D = 15$  nm. a) I-V, b) Responsivity, c) Asymmetry, d) Transmittivity spectrum (T) at  $1.76$  V of voltage bias, for  $w = 1$  nm,  $L = 12$  nm,  $D = 15$  nm.

**C. EXTENDING THE DIODE GEOMETRY**

In the following, charge ballistics is still assumed to explore the impact of diode topology on I-V curves. In particular, two additional geometries have been considered. As a first

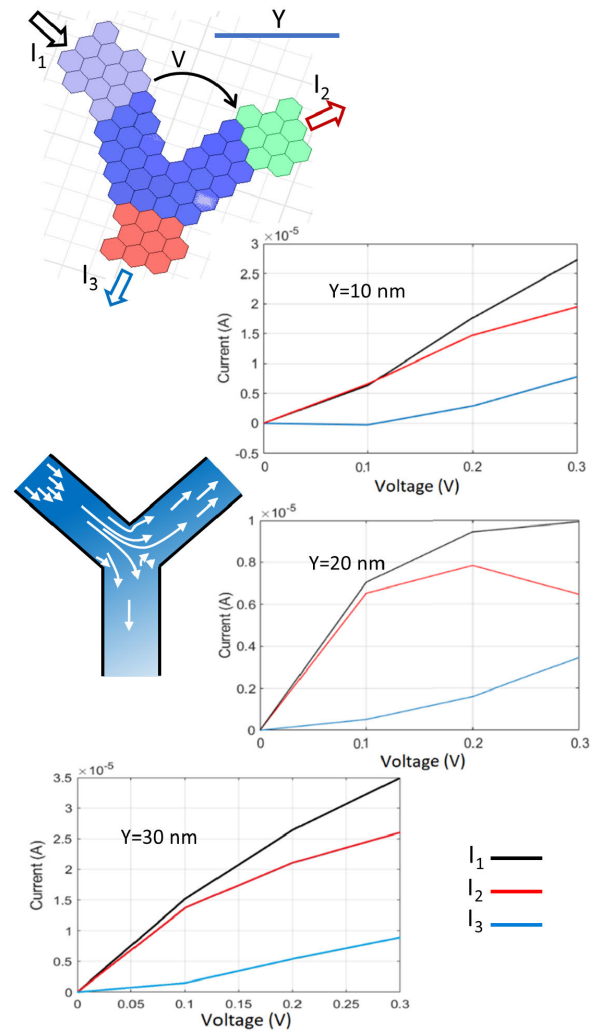
case, we evaluate the effect of cascading graphene tapers to see if this could provide significant benefit to the I-V response. As a result, the current obtained by two consecutive apertures is significantly lower than the one obtained with a



**FIGURE 8.** The top picture shows the I-V curves obtained with one and two asymmetric apertures, respectively in blue and orange; in the inset the asymmetry calculated for the two cases.

single aperture, despite charge ballisticity, and I-V asymmetry does not seem to benefit from the reduced reverse current (absolute value) since the forward current reduces accordingly. Results and geometric details are shown in Fig. 8. The parallel of geometric diodes has not been considered here, as it is expected to bring larger reverse current which is likely to make any rectification much less effective. As a secondary point, having parallel asymmetries would require a significant increase of numerical complexity, as the graphene section would increase, with a corresponding increase in the number of electronic channels above cutoff.

The other case considered here is a 3-port graphene circuit, or Y-junction, in contrast to the case of the 2-port circuits analyzed until now. A sinusoidal voltage  $V$  between two ports (1 and 2) results, due to charge ballisticity, in a nonzero current at port 3, where charges are assumed to be perfectly absorbed (ideal perfect matching). In this way, (at least partial) rectification of the voltage between port 1 and 2 could be achieved at port 3. Geometry and numerical results are shown in Fig. 9. Such an effect, which is not possible in classical or diffusive pictures, has been quantified basing on the simulation of the scattering parameters among three multichannel ports. Simulation is done for the specific chirality (armchair) of the graphene branches, as indicated in Fig. 9. The latter also shows that, in general, a relatively small fraction of the current entering port 1 can be delivered out of port 3. However, an interesting point could be remarked: the effect of the asymmetry is higher at higher voltages, where the current  $I_3$  reaches up to 20% – 30% of



**FIGURE 9.** I-V characteristic of a graphene Y-junction, for different sizes.

the input current  $I_1$ . It will be interesting to see, in a next development of this work, if this trend is maintained even for higher voltages and for larger structures, which is currently under numerical test. In that case, the behavior of the 3-port circuit would be opposite to the one of the previous 2-port circuits, and a proper combination of these geometries could be used to engineer the I-V response. It is remarked that, in general, numerical post-processing is crucial to extract the scattering parameters between the electronic channels at any considered contact (port) of the graphene circuit. Depending on the size of computational domain, one single point of the I-V curves at high voltages could take up to 10 h - 20 h (tens of thousands of atoms) and several GB RAM. However, post-processing allows easy combination of several sub-modules to describe much larger and complex structures (in principle, up to hundreds of thousands of atoms, but the actual number is always a compromise with numerical accuracy). In this way, cascaded diodes and 3-port junctions could be evaluated. 4-port circuits are currently under consideration.

#### IV. CONCLUSION

In this paper, geometrical planar diodes based on graphene are numerically simulated to investigate the main features of their current-voltage (I-V) response, in view of applications to optical rectennas and nano-patterned antenna arrays. Coherent charge transport is analyzed to properly capture the quantum effects related to charges propagation, that is, reflection/transmission, interference, and tunneling. In recent years, I-V asymmetry and related figures of merit have been discussed by several Authors for graphene geometric diodes, but the present contribution distinguishes from previous ones in two main respects. First, we propose a rigorous analysis of charge transport extending in-house software based on Scattering Matrix method (SM) to highlight the impact of geometric and physical parameters on diode output, to be possibly used as general guidelines for design. Besides, we start to generalize our study to more complex structures, such as cascaded two port asymmetries and three port devices, where the size of the scattering matrix rapidly increases to account for the high number of electronic channels involved. We believe that the above approach could lead, in a next development of this work, to better and optimized topologies of electromagnetic rectifiers, not necessarily limited to two-port geometries. This could help to overcome the current limits in terms asymmetry and nonlinearity, that still prevent from an effective implementation of the concept of geometric diode for harvesting applications.

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#### DISCLOSURES

The authors declare no conflicts of interest.

#### DATA AVAILABILITY STATEMENT

Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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