# COMPARING GRAPHENE ENERGY DISPERSION SIMULATIONS USING SPREADSHEET FOR DISTANCE LEARNING

## COMPARACIÓN DE SIMULACIONES DE DISPERSIÓN DE ENERGÍA DEL GRAFENO UTILIZANDO UNA HOJA DE CÁLCULO PARA EL APRENDIZAJE A DISTANCIA

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This study aims at simulating the energy dispersion of graphene using Spreadsheet as a distance (online) learning as a solution for physics learning, especially for undergraduate students. Here we compare the simulation results of graphene's dispersion energy from various literatures and then discussed them from the educational point of view. The Spreadsheet is used to visualize the energy dispersions of graphene having hexagonal honeycomb lattice structure. The results obtained are graphene's energy dispersion simulations from various literature sources, especially from 2010 to 2019. Moreover, although the mathematical formulas are different, the graphene's energy dispersion profiles are mostly similar in wireframe and 3D surface patterns. These simulation results can be used in teaching undergraduate students in making simple simulations using Spreadsheet.

Este estudio tiene como objetivo simular la dispersión de energía del grafeno utilizando hoja de cálculo como una solución de aprendizaje a distancia (en línea) para aprender física, especialmente para estudiantes de pregrado. Aquí comparamos los resultados de la simulación de la energía de dispersión del grafeno de diversas publicaciones y luego lo discutimos desde la perspectiva educativa. La hoja de cálculo se utiliza para visualizar la dispersión de energía del grafeno con una estructura de celosía de panal hexagonal. Los resultados obtenidos son simulaciones de dispersión de energía del grafeno de diversas fuentes de la literatura, especialmente de 2010 a 2019. Además, aunque las fórmulas matemáticas son diferentes, los perfiles de dispersión de energía del grafeno son en su mayoría similares a patrones de estructura wireframe y superficies 3D. Estos resultados de la simulación se pueden utilizar para enseñar a los estudiantes universitarios a realizar simulaciones sencillas con la hoja de cálculo.

PACS: Graphene (grafeno), 81.05.ue; surface states, band structure, electron density of states (estados de superficie, estructura de bandas, densidad de electrones de estados), 73.20.At; computer modeling and simulation (modelado y simulación por computadora), 07.05.Tp; education (educación), 01.40.d.

## I. INTRODUCTION

In the recent past, we have faced a pandemic situation. However, the learning process in universities must continue. Many universities have shifted from face to face lectures to online or distance learning clases to minimize the spread of COVID-19 [1]. However, an obstacle in the field is that only few students tend to enjoy the distance learning process [2].

In education, especially university or college level, the introduction of various materials in the field of physics is still lacking. For example, students may not know that pencils are made of graphite. Interestingly, graphite consists of many layers of graphene. Graphene is a two dimension (2D) material consisting of carbon atoms with hexagonal honeycomb lattice [3, 4]. Graphene has physical properties that are of interest to physics and other applications. Graphene can create 2D structures from different chemical compositions such as nitogen boride [5]. Graphene can be wrapped into 0 dimension (0D) fullerenes, rolled in a certain direction into one dimension (1D) carbon nanotubes (CNT), and stacked layer by layer into three dimensions (3D) graphite in pencils. The flexibility of the graphene structure gives its many interesting properties [6]. All this makes graphene an interesting topic for university level.

An interesting physical property of graphene, which is important to be studied is its electronic band structure. The electronic band structure of graphene consists of Dirac points, where the valence and conduction bands converge. The cone shape of the energy band structure shows linear electronic dispersion and density of state (DOS) [7]. There are several methods that can be applied to determine the electronic band structure of graphene. One of them is using the tight binding method [8]. This method determines the energy dispersion as a function of the k-wave [9]. Some of the energy dispersion formulas for graphene using the tight binding method are presented in equations (1) to (14). These formulas are explicitly contained in articles, which are obtained from 2010 to 2019. These formulas can be seen in Table 3.

Most of these formulas have been simulated using Matlab software. However, in this study, we use Spreadsheet. This is because Spreadsheet can be used to analyze and visualize data. Spreadsheet is a user-friendly software. Many scientists have used Spreadsheet to simulate topics of physics and other disciplines [9–16]. Spreadsheet does not require complex programming and students know how to operate the software [12,13].

This study aims to simulate the energy dispersion of graphene using Spreadsheet as a distance learning solution for learning physics, especially for undergraduate students. In addition, we also compare the simulation results of graphene's dispersion energy from various literatures and discussed them from the educational perspective.

## II. RESEARCH METHOD

Table 1. Spreadsheet formula for Moreau's (2016) graphene energy dispersión of the E(+) part.

| Cell | Parameter | Formula |
|---|---|---|
| A2 | Lattice constant | =2.46 |
| B2 | Hopping parameters | =2.8 |
| C2 | | = 0.2*$B$2 |
| C5-BB5 | x-axis | Range (-2.55414 ; 2.54586), interval 0.1 |
| B6-B57 | y-axis | Range (-2.55414 ; 2.54586), interval 0.1 |
| C6-BB57 | Energy dispersion | =$B$2*SQRT(3+2*COS (SQRT(3)*C$5*$A$2)+ 4*COS(SQRT(3)/2*C$5*$A$2) COS(3/2*$B6*$A$2))- $C$2*(3+2*COS(SQRT(3)* C$5*$A$2)+4*COS(SQRT (3)/2*C$5*$A$2)*COS(3/2* $B6*$A$2)) |

Table 2. Spreadsheet formula for Moreau's (2016) graphene energy dispersión of the E(-) part.

| Cell | Parameter | Formula |
|---|---|---|
| A2 | Lattice constant | =2.46 |
| B2 | Hopping parameters | =2.8 |
| C2 | | = 0.2*$B$2 |
| C5-BB5 | x-axis | Range (-2.55414 ; 2.54586), interval 0.1 |
| B6-B57 | y-axis | Range (-2.55414 ; 2.54586), interval 0.1 |
| C6-BB57 | Energy dispersion | =-$B$2*SQRT(3+2*COS (SQRT(3)*C$5*$A$2)+ 4*COS(SQRT(3)/2*C$5*$A$2) COS(3/2*$B6*$A$2))- $C$2*(3+2*COS(SQRT(3)* C$5*$A$2)+4*COS(SQRT (3)/2*C$5*$A$2)*COS(3/2* $B6*$A$2)) |

The Spreadsheet is used to visualize the energy dispersion of graphene with hexagonal honeycomb lattice structure. The first step is to determine the parameters of the formulas in Table 3. The lattice constant used is 2.46 Å. The wave number, k, for the x and y-axes, i.e.: kx and ky, respectively, are in the range of $-2\pi$a to $2\pi$a with an interval of 0.1. Meanwhile, the kz value is 0 because graphene is a 2D structure. Complete parameters for simulating the positive and negative energies, i.e.: E(+) and E(-) parts of graphene's energy dispersión can be seen in Tables II and III, respectively. The energy dispersion represented in Tables II and III is the equation given by Moreau (2016). The energy dispersion is obtained from the relationship between the x and y-axes by paying attention to the equations in Table 3.

Fig. 1 shows Moreau's (2016) Spreadsheet analysis for graphene's energy dispersions for the E(+) and E(-) parts. The mathematical equations (1) to (14) are entered in the Spreadsheet so that the distribution of values from $-2\pi$a to $2\pi$a is obtained.

## III. RESULTS AND DISCUSSION

The parameter that is kept constant in the study is a = 2.46 Å, with the range for $k_x$ and $k_y$ are $-2\pi$a to $2\pi$a, and interval for $k_x$ and $k_y$ is 0.1. The energy dispersion profiles contain two parts, namely positive (up) and negative (down) parts. This happens because of the plus-minus sign in all equations in Table 3. The Spreadsheet cannot display 3D positive and negative curves at the same time. To overcome this, a contour wireframe is used. This feature is used to visualize the equation and find out the difference between each energy dispersion pattern. The contour wireframe can bring out a 2D appearance from the original 3D shape. In this case, one energy dispersion equation has to be split into the positive [E(+)] and negative [E(-)] parts to get the patterns.

Various explicit and closed formulas for graphene's dispersion energies may be observed in Table 3, i.e.: equations (1) to (14). It may be observed that these equations look different with various parameters. Some of these equations have been produced using Matlab. It may also be noted that there are some errors in the formula, especially in equations (1) and (13). This error can be seen from the curve formed and the absence of an x-axis in each equation. We know that graphene is 2D, so that the axis used is not only the y-axis but also the x-axis. We also have given the correct version of the equations below each incorrect formula.

It can also be explicitly observed that there are differences in the use of the parameter a, namely 1.42 Å for equations (1), (6), (9), (10), and (11), and 2.46 Å for the equations (2), (3), (5), and (8). In this case, two examples of simulation results that illustrate the difference in parameter "a" are given in Fig. 2 using the same equation, namely equation (11). It can be observed in Fig. 2 that the range of values obtained for the energy dispersion is still the same. The difference is the number of cone shapes of the Dirac points.

Moreover, we provide the simulation results of graphene's dispersion energies for a total of 14 equations given in Table 3. The simulations are obtained using Spreadsheet via wireframe contour for E(+) and E(-). The simulations results are given in

Fig. 7.

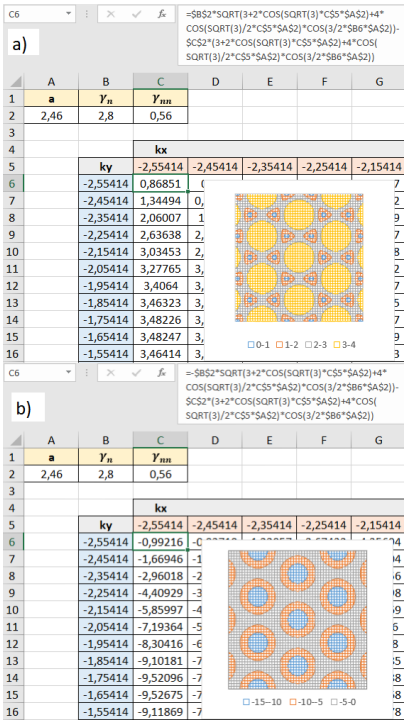


Figure 1. Spreadsheet analysis for Moreau's (2016) graphene energy dispersion for a) E(+) and b) E(-).

These results indicate that the energy dispersion equations proposed by several authors have similar patterns, such as the patterns given by equations (1), (3) to (6), (9), (11), (12), and (14). From these patterns, then we may also look at different profiles through the 3D surface. But, the energy dispersion curves must still be separated into two parts, that is E(+) and E(-). These are given in Figs. 8 and 9, respectively. Especially for equation (4), the E(+) part is not presented in Fig. 8 because the 3D surface profile produces different pattern. Hence, only the E(-) part of equation (4) is given in Fig. 9. The rotation angle for each curve is the same, that is 60° and 20° for the X- and Y-rotations, respectively, so that the cones of each pattern are clearly observed.

From Fig. 8 it can be observed that the shape of E(+) of these equations is relatively the same. The only difference is the range of the energy dispersion values and the number of the Dirac points. There is another characteristic that stands out from equation (1), especially the E(+) pattern. Compared to the other patterns, the E(+) of equation (1) has a cone shape that is flatter on the x-axis. Furthermore, Fig. 9 below is the pattern of the E(-) for each equation.

From Fig. 9, it can be observed that the shape of E(-) is of two distinct patterns. The first group consists of equations (1), (6), (9), (11), (12), and (14). The characteristic of this group is that it has a pair of cones that is close together. The least number of cones is given by equation (1), while the other equations have the same number of cones. The second pattern consists of equations (3), (4), and (5), which has a six flower petal-like cone shape. At a specific $k_x$ and $k_y$, this pattern only forms one flower petal arrangement consisting of six cone shapes. The shallowest of these cone shapes is given by equation (4).

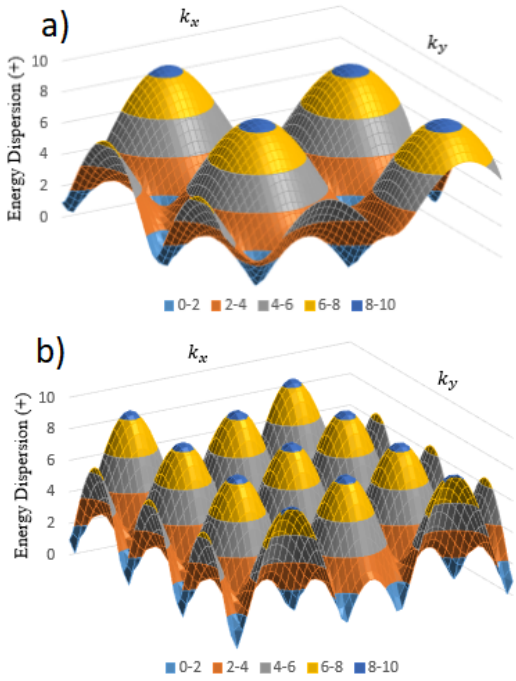


Figure 2. Sjolander's (2017) E(+) part with a) a = 1.42 Å and b) a = 2.46 Å.

Brocks (2015) actually have a similar pattern to Figs. 8 and 9, but it is relatively slanted, pointed, and seemingly stretched making the patterns look different. Besides that, Brocks' (2015) pattern is also inverted, i.e.: when the value of E is positive and negative, the curve is below and above the origin, respectivley. This anomaly can be observed in Fig. 3.

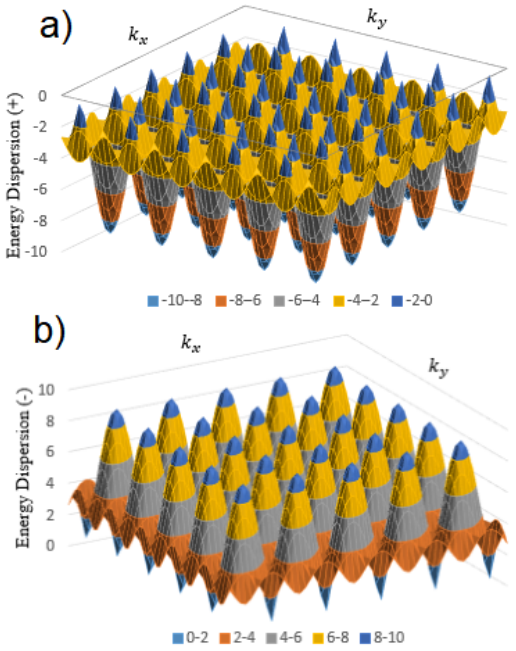


Figure 3. Brocks' (2015) energy dispersion parts, i.e.: a) E(+) and b) E(-).

The patterns that are different from the majority of the energy dispersion patterns are given by equations (2), (4), (8), and (13). Equation (2) is given by Fathi (2011). Based on the wireframe contour, it is observed that equation (2) does not directly show a hexagonal structure. The observation made using the 3D surface shows that there is a similarity between Fathi's (2011) pattern and E(+) pattern of equations (1), (3) to (6), (9), (11), (12), and (14). However, the low values of the energy dispersion and the cones that do not form a hexagonal structure at the specified $k_x$ and $k_y$ resulted in a different pattern when observed using the wireframe contour. This can be seen in Fig. 4.

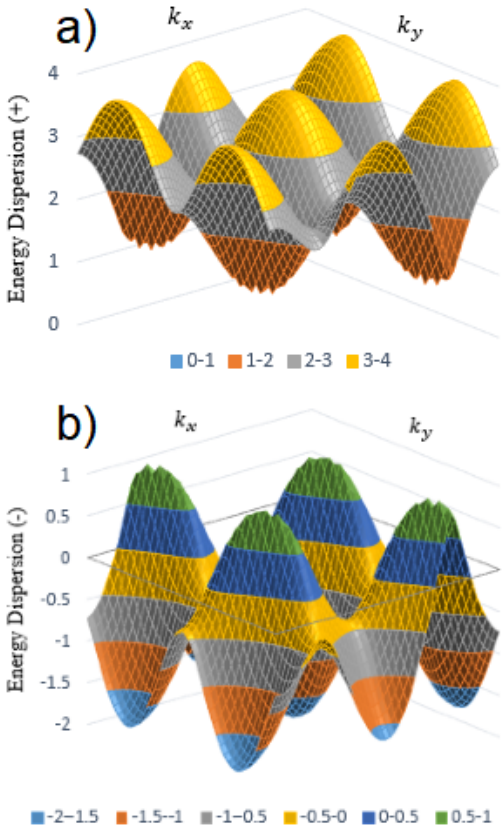


Figure 4. Fathi's (2011) energy dispersion parts with a) E(+) and b) E(-).

Moreau's (2016) and Armano's (2019) energy dispersion patterns have the same E(-) but differ from the majority of other E(-) patterns. To see in more detail, the E(-) patterns are simulated using the contour and 3D surface, which may be observed in Fig. 5. It can be seen that the pattern formed by Moreau's (2016) and Armano's (2019) also show a hexagonal structure. The pattern formed using the 3D surface is also similar to equations (1), (6), (9), (11), (12), and (14).

Finally, Kolb's (2012) E(+) pattern has the lowest value. This can be seen from the low values of the energy dispersion of the 3D surface in Fig. 6. This equation is considered poor because it cannot display a high enough energy dispersion values. If the observation is carried out using the wireframe contour, the energy dispersion pattern is very different from the majority of other patterns (see Fig. 7 above).

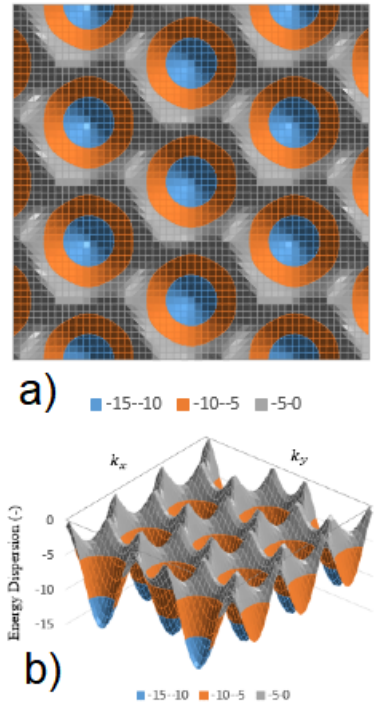


Figure 5. Moreau's (2016) and Armano's (2019) energy dispersions of the E(-) part with a) contour surface and b) 3D surface.

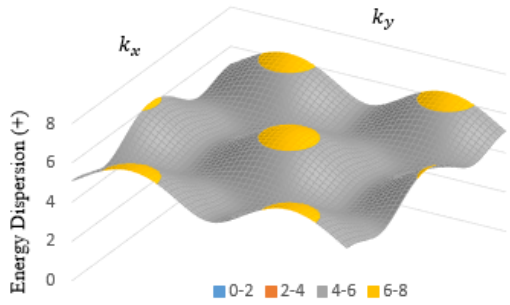


Figure 6. Kolb's (2012) energy dispersion of the E(+) part.

From this study, we can discuss the advantages and disadvantages of Spreadsheet in visualizing the energy dispersion of graphene. The advantage of the Spreadsheet is that it does not require complex programming to visualize the energy dispersion equation. As long as the parameters and mathematical equations are complete, a graph of the energy dispersion can be formed easily and quickly. Visualization can be done using a contour, wireframe contour, or 3D surface in the Spreadsheet menu chart. The use of these three features can be very helpful in visualizing the shape of the energy dispersion. Meanwhile, the weakness of Spreadsheet is that it cannot visualize E(+) and E(-) curves at one time. The graphene dispersion energy equation must be broken down into two parts to get the patterns.

The above results can be used in an online learning. This

may go as follows. First, students are given a task to look for articles concerning pencils. The article should contain an explanation of the constituent materials of pencils, the differences between graphene and graphite, the benefits of studying graphene, and several graphene energy dispersion equations using the tight binding method. Then, the students are asked to study the mathematical form of the energy dispersion equations without having to derive them as it only uses simple trigonometric function. Finally, the students are asked to simulate the equations using Spreadsheet.

Spreadsheet does not require complex programming so that students can feel the ease to use it. Making simulations using Spreadsheet makes the distance (online) learning fun during the COVID-19 pandemic. A benefit of making simulation is that students can easily understand the concept of the material being studied [26,27]. In addition, the unique patterns of graphene's energy dispersion using contour, wireframe contour, and 3D surface are also interesting to study. Students are asked to explain the similarities and differences in the patterns that are formed. The purpose of this activity is that students realize that the objects around them are composed of unique and interesting materials that can be simulated simply using a Spreadsheet. Studying the unique properties of materials will be useful for students' further study. University students and experts can also use this simulation for research concerning the formulation of Dirac points, which is useful in understanding the benefit in not having band gaps in graphene.

## IV. CONCLUSION

In this study, we have simulated graphene's energy dispersion based on various literature sources from 2010 to 2019. All simulations are made using Spreadsheet. In general, the mathematical form of the energy dispersion equations are different. However, most of these equations produce similar simulation results of honeycomb hexagonal structure with Dirac points in wireframe and 3D surface patterns. The results of this simulation can be used in teaching undergraduate students about the energy dispersion of graphene. In addition, students may also be encourage to make simple simulations using Spreadsheet.

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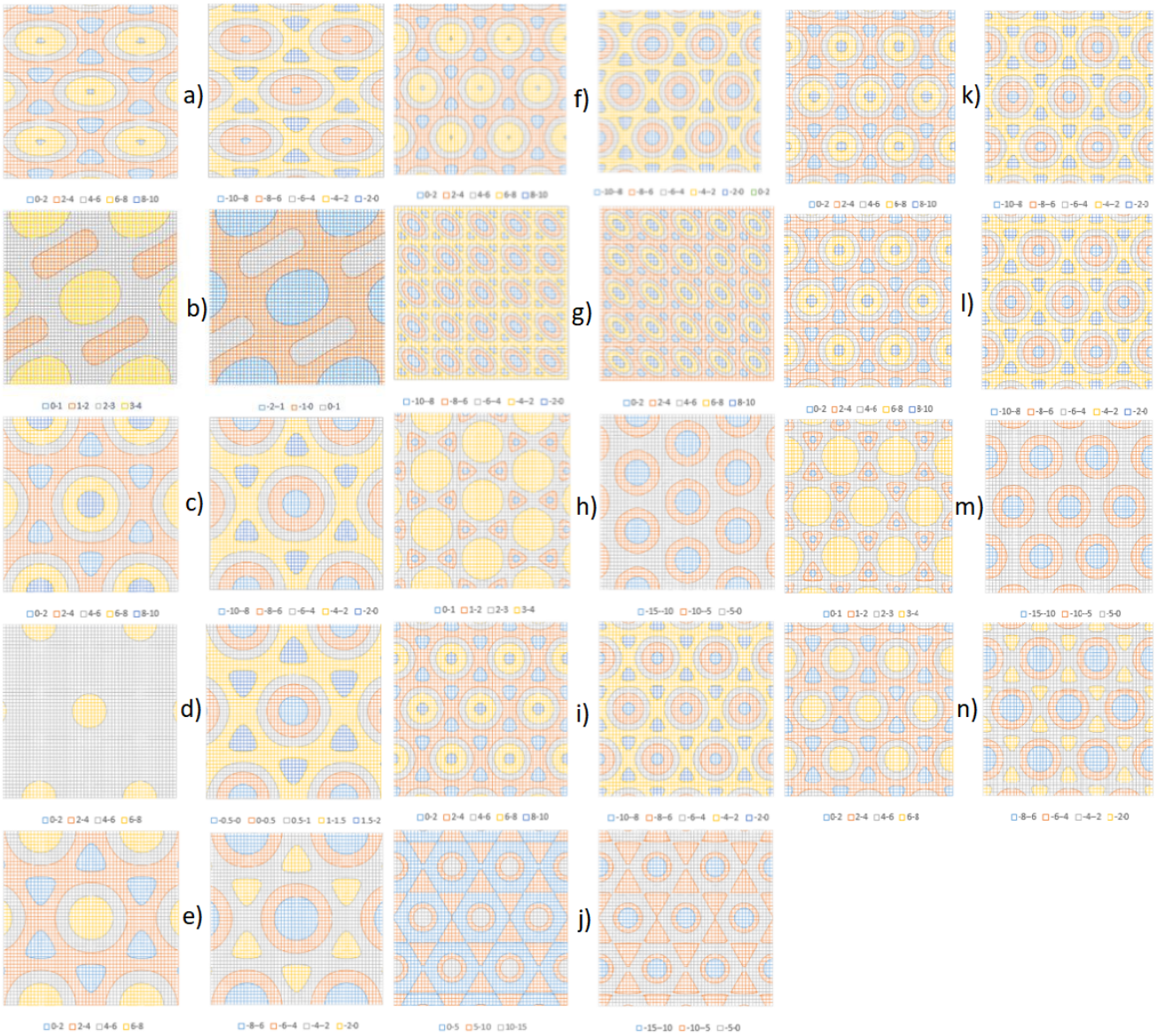


Figure 7. Graphene energy dispersion for a) Luo (2010); b) Fathi (2011); c) Aydin, et al (2011)' d) Kolb (2012); e) Muoth (2013); f) Kadirko (2013); g) Brocks (2015); h) Moreau (2016); i) Zhu, et al (2016); j) Rozhkov, et al (2016); k) Sjolander (2017); l) Utermohlen (2018); m) Armano, et al (2019); and n) Adhikary, et al (2019).

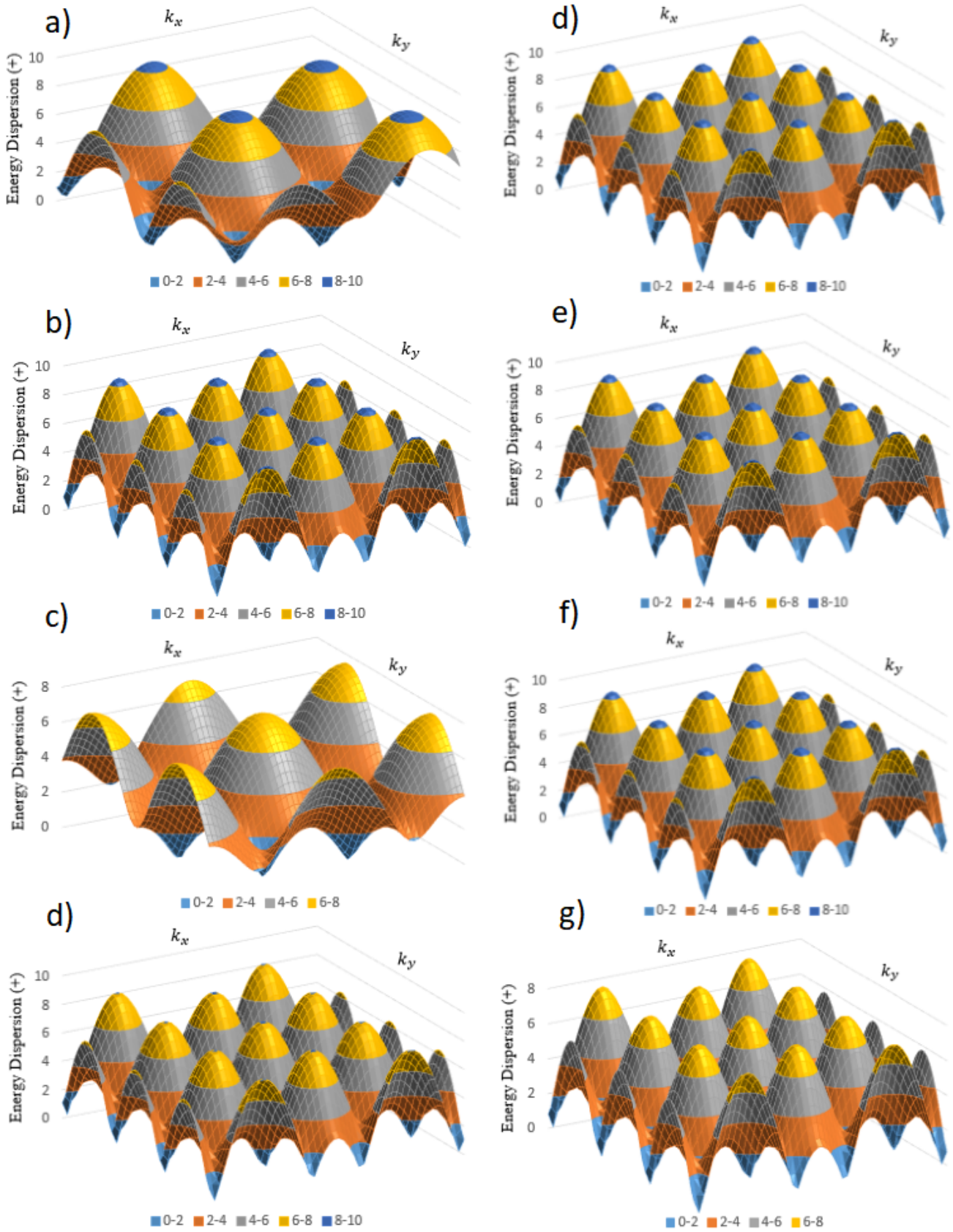


Figure 8. Graphene's energy dispersion of E(+) from a) Luo (2010); b) Aydin, et al (2011); c) Muoth (2013); d) Kadirko (2013); e) Zhu, et al (2016); f) Sjolander (2017); g) Utermohlen (2018), and h) Adhikary, et al (2019).

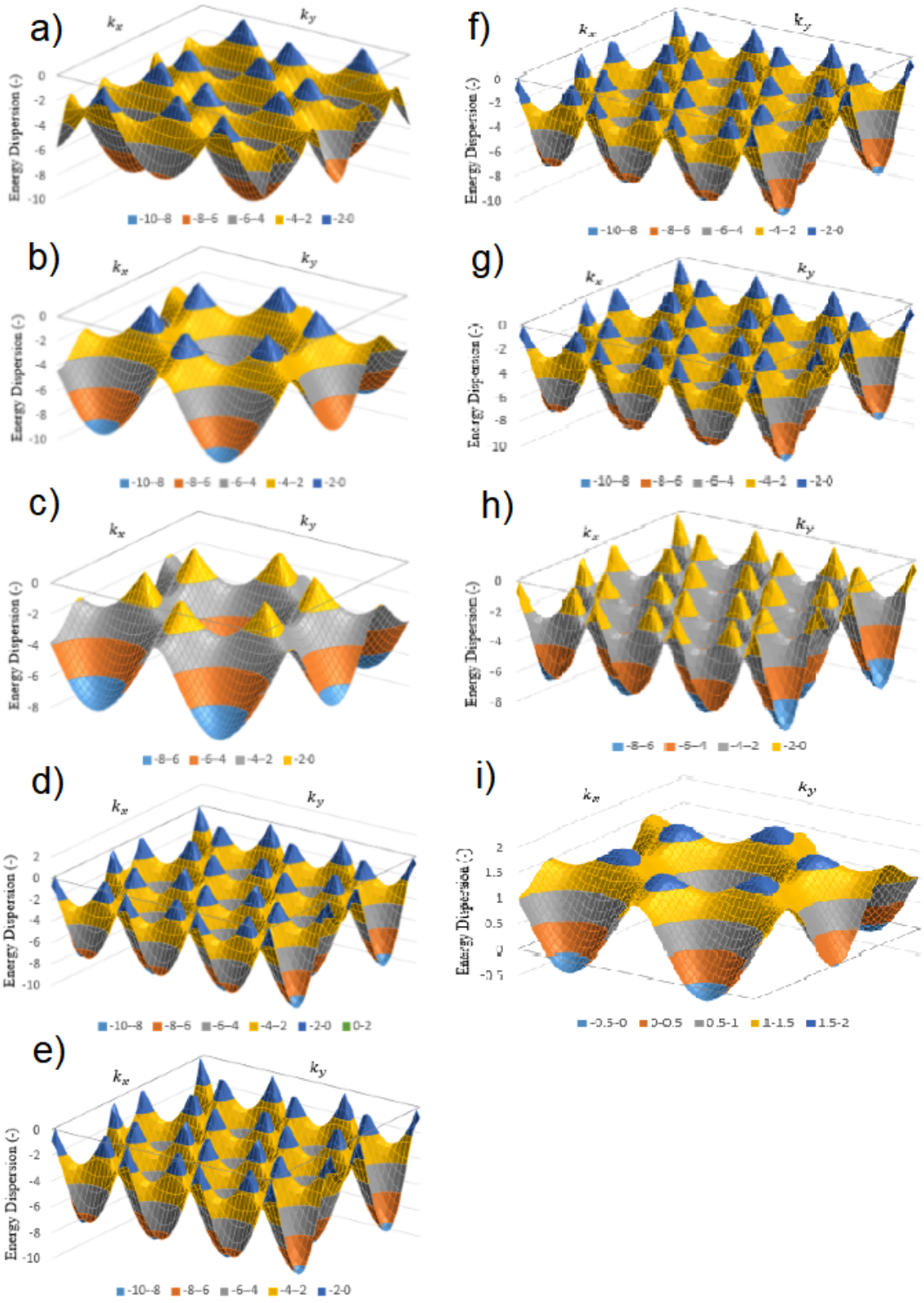


Figure 9. Graphene's energy dispersion of E(-) from a) Luo (2010); b) Aydin, et al (2011); c) Muoth (2013); d) Kadirko (2013); e) Zhu, et al (2016); f) Sjolander (2017); g) Utermohlen (2018); h) Adhikary, et al (2019) and i) Kolb (2012).

Table 3. Graphene's energy dispersion formulas

| Author | Equation | Parameters | Software |
|---|---|---|---|
| Luo [6] | $E(k) = \mp t_1 \sqrt{3 + f(\vec{k})} - t_2 f(\vec{k})$ (1)<br>$f(\vec{k}) = 2cos(\sqrt{3}ak_y) + 4cos(\frac{\sqrt{3}}{2}ak_y)cos(\frac{\sqrt{3}}{2}ak_y)$<br>Note: the equation is wrong, it should be $cos(\frac{\sqrt{3}}{2}ak_x)$ not $cos(\frac{\sqrt{3}}{2}ak_y)$ | a≈1.42 Å<br>t1=2.7 eV<br>t2=0 | - |
| Fathi [15] | $\epsilon = \alpha \mp \beta \sqrt{3 + cos(\frac{a}{2}(\sqrt{3}k_x + k_y)) + 2cos(\frac{a}{2}(\sqrt{3}k_x - k_y)) + 2cos(ak_y)}$ (2) | a=2.46 Å | Matlab |
| Aydin, et al [16] | $E(k) = \mp\gamma \sqrt{3 + 2[cos(\vec{k}\cdot\vec{a_1}) + cos(\vec{k}\cdot\vec{a_2}) + cos(\vec{k}\cdot\vec{a_1} - \vec{k}\cdot\vec{a_2})]}$ (3)<br>$\vec{k} = k_x\hat{x} + k_y\hat{y}$<br>$E(k) = \mp\gamma \sqrt{3 + 2[cos\frac{a}{2}(\sqrt{3}k_x + k_y)) + cos(\frac{a}{2}(\sqrt{3}k_x - k_y)) + cos(ak_y)]}$ | a= $\sqrt{3}a_{cc}$<br>$a_{cc}$=0.142 nm<br>$\gamma$=2.9∓0.2 eV | - |
| Kolb [17] | $\frac{(\epsilon_B+\epsilon_N)}{2} \mp \sqrt{\frac{(\epsilon_B-\epsilon_N)^2}{2} + 4t^2[(cos(\frac{k_y}{2}a))^2 + cos(\frac{\sqrt{3}k_y}{2}a)cos(\frac{k_y}{2}a) + \frac{1}{4}]}$ (4) | $\epsilon_B$=4<br>$\epsilon_N$=2.1<br>t=1 | Matlab GUI |
| Muoth [18] | $E = E_o \mp \gamma_o \sqrt{1 + 4cos(\frac{\sqrt{3}k_x a}{2})cos(\frac{k_y a}{2}) + 4cos^2(\frac{k_y a}{2})}$ (5) | a=0.246 nm<br>$E_o$= 0 eV<br>$\gamma_o$=2.5-3.3 eV | Matlab |
| Kadirko [19] | $E(k) = \mp t \sqrt{3 + f(k)} - t' f(k)$ (6)<br>$f(k) = 2cos(\sqrt{3}k_y a) + 4cos(\frac{\sqrt{3}}{2}k_y a)cos(\frac{3}{2}k_x a)$ | a=1.42 A<br>t=2.8 eV<br>t'=0.02t-0.2t | - |
| Brocks [20] | $E_k = E_p \mp t \sqrt{3 + 2cos(2\pi k_1) + 2cos(2\pi k_2) + 2cos(2\pi(k_1 + k_2))}$ (7)<br>Note: $k_1 = k_x$ dan $k_2 = k_y$ | $E_p$=0<br>t≈-3 eV | - |
| Moreau [4] | $E = \mp\gamma_n \sqrt{3 + f(k)} - \gamma_{nn} f(k)$ (8)<br>$f(k) = 2cos(\sqrt{3}k_x a) + 4cos(\frac{3}{2}k_x a)cos(\frac{3}{2}k_y a)$ | a=2.46 Å<br>$\gamma_n$=2.8<br>$\gamma_{nn}$=0.2$\gamma_n$ | Matlab |
| Zhu, et al [21] | $E(k) = \mp t \sqrt{3 + 2cos(\sqrt{3}k_y a) + 4cos(\frac{\sqrt{3}}{2}k_y a)cos(\frac{3}{2}k_x a)}$ (9) | a≈1.42 Å<br>t=2.8 eV | Matlab |
| Rozhkov, et al [5] | $\epsilon_k = \mp t\|f(k)\|$ (10)<br>$f(k) = 2cos(\sqrt{3}k_y a_o) + 4cos(\sqrt{3}k_y a_o/2)cos(3k_x a_o/2)$ | $a_o$=1.42 Å<br>t=2.5-3 eV | - |
| Sjolander [22] | $E(k) = \mp h_o \sqrt{\|f(k)\|^2} - h_1\|f(k)\|^2$ (11)<br>$\|f(k)\|^2 = 3 + 4cos(\frac{\sqrt{3}}{2}k_y a_{c-c})cos(\frac{3}{2}k_x a_{c-c}) + 2cos(\sqrt{3}k_y a_{c-c})$ | $a_{c-c}$=1.42 Å<br>$h_o$=2.8 eV<br>$h_1$=0 | Matlab |
| Utermohlen [23] | $E(k) = \mp t \sqrt{1 + 4cos(\frac{3}{2}k_x a)cos(\frac{\sqrt{3}}{2}k_y a) + 4cos^2(\frac{\sqrt{3}}{2}k_y a)}$ (12) | - | - |
| Armano, et al [24] | $E = \frac{\epsilon_{2pz} \mp t\sqrt{\|f(k)\|}}{1 \mp s\sqrt{\|f(k)\|}} \approx \epsilon_{2pz} \mp t\sqrt{\|f(k)\|} - s\|f(k)\| + ...$ (13)<br>$f(k) = 1 + 4cos(\frac{\sqrt{3}}{2}k_y a)cos(\frac{3}{2}k_y a) + 4cos^2(\frac{\sqrt{3}}{2}k_y a)$<br>Note: the equation is wrong, it should be $cos(\frac{3}{2}k_x a)$ not $cos(\frac{3}{2}k_y a)$ | a=1.42 Å<br>t=2.7 eV<br>s=0.2t<br>$\epsilon_{2pz}$=0 | - |
| Adhikary, et al [25] | $\epsilon = \mp\gamma_o \sqrt{1 + 4cos(k_x \frac{3a}{2})cos(k_y \frac{\sqrt{3}a}{2}) + 4cos^2(k_y \frac{\sqrt{3}a}{2})}$ (14) | $\gamma_o$=2.5-3 eV | Matlab |