The misconception in graphene's dispersion energy simulations

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This study aims to find equations and simulations that satisfy the characteristics of graphene's energy dispersion and identify misconceptions that may occur. Here we give students nine articles about graphene's dispersion energy. They were asked to identify the equations, parameters, and software used in each of the articles. The assignment was then to make the distribution of the data in a spreadsheet. The parameters used were the lattice constant of 2.46 Å, the range of the k wave function for the x and y axes of $-2\pi a$ to $2\pi a$, and the interval for each range of 0.1. Each equation is divided into two parts, $E(+)$ and $E(-)$. The analysis was carried out by making a slice in the middle of the x and y axes, as well as the main and off-diagonals. Graphene has Dirac points where the band gap is zero. This means that there is no distance or very small distance between the valence and conduction bands. From this activity, it can be concluded that Rozhkov (2016) has the equations and simulations that best satisfy graphene's dispersion energy. Misconceptions occur in almost all existing equations and simulations.

Keywords: Dispersion energy; graphene; simulations; distance learning; spreadsheet.

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1. Introduction

The Covid-19 pandemic demands interesting and fun distance learning. Such learning must be directed towards meaningful learning. The introduction of Material courses in the pandemic era can be done by introducing materials related to the lives around students [1]. Graphene is a material that is discussed a lot these days. Graphene comes from single-layer graphite [2]. Graphite can be found, *e.g.*: in pencil [3]. In the last decade, many articles have discussed equations and simulations of graphene's dispersion energy. These articles contain graphene's dispersion energy equation, although they produced different equations and simulations. The interesting thing here is that we can ask students to find equations and simulations that satisfy the characteristics of graphene's energy dispersion and identify misconceptions that may occur. This research is important because the simulations produced in the previous articles cannot show the Dirac points as they are drawn in 3D so that some parts of the Dirac points may not be directly apparent. This makes it difficult to distinguish equations and simulations according to the graphene's dispersion energy characteristics.

The spreadsheet software is used in this activity. The reason is that students are familiar with spreadsheets and spreadsheets do not require complex programming [4,5]. Moreover spreadsheets can also be used to identify misconceptions [6].

Graphene is a 2D material consisting of hexagonal or honeycomb-shaped carbon atoms [7,8]. There are two groups of energy levels or orbitals, the bottom is called the valence band and the top is called the conduction band [9]. Dirac point is the meeting point between the valence band and the conduction band in graphene. Graphene has a bandgap close to or equal to zero. Graphene can be made from graphene oxide (GO). GO has a bandgap proportional to the oxygen atoms' concentration. If the degree of oxidation increases, the bandgap opens and GO has properties like an insulator. The bandgap in GO is greater than zero [10, 11].

In this article, we will discuss nine equations of graphene's dispersion energy. The nine equations are in Eq. (1). The analysis was carried out by making a slice in the middle of the x and y axes, as well as the main and off-diagonals. These nine equations were chosen because they have different shapes of the dispersion energy so that they are interesting for further studies.

2. Method

The learning method was that students were given nine articles about graphene's dispersion energy. They were asked to identify the equations, parameters, and software used in each of the article. The assignment was then to make the distribution of the data in a spreadsheet as shown in Fig. 1. The parameters used were the lattice constant of 2.46 Å, the range of the k wave function for the x and y axes of $-2\pi a$ to $2\pi a$, and the interval for each range of 0.1. Each equation is divided into two parts, namely $E(+)$ and $E(-)$. Students were asked to make data slices and curves in the middle of the x-axis ($\pm 0.05; k_y$) in orange-colored cells (Fig. 1), the center of the y-axis (k_x; ± 0.05) in blue-colored cells (Fig. 1), main diagonal ($k_x; k_y$) in yellow-colored cells (Fig. 1), and off diagonal ($k_x; -k_y$) in dark pink-colored cells (Fig. 1). The aim is to make it easier to observe the Dirac point and energy gap for each of the equations. Examples of the spreadsheet formulas for the Rozhkov (2016) equation are shown in Table II and III.

TABLE I. Graphene's energy dispersion formulas.

Author	Equation	Parameters	Software
Luo [12]	$E(k) = \pm t_1\sqrt{3+f(\vec{k})} - t_2 f(\vec{k})$ $f(\vec{k}) = 2\cos\left(\sqrt{3}ak_y\right) + 4\cos\left(\frac{\sqrt{3}}{2}ak_x\right)\cos\left(\frac{\sqrt{3}}{2}ak_y\right)$	$a \approx 1.42$ Å $t_1 = 2.7$ eV $t_2 = 0$ eV	-
Fathi [2]	$\mathcal{E} = \alpha \pm \beta\sqrt{3+\cos\left(\frac{a}{2}\left(\sqrt{3}k_x+k_y\right)\right)+2\cos\left(\frac{a}{2}\left(\sqrt{3}k_x-k_y\right)\right)+2\cos\left(ak_y\right)}$	$a = 2.46$ Å	Matlab
Aydin, *et al* [13]	$E(k) = \pm\gamma\sqrt{3+2\left[\cos\left(\frac{a}{2}\left(\sqrt{3}k_x+k_y\right)\right)+\cos\left(\frac{a}{2}\left(\sqrt{3}k_x-k_y\right)\right)+\cos\left(ak_y\right)\right]}$	$a = \sqrt{3}a_{cc}$ $a_{cc} = 0.142$ nm $\gamma = 2.9 \pm 0.2$ eV	-
Kolb [14]	$E = \frac{(\varepsilon_B+\varepsilon_N)}{2} \pm \sqrt{\frac{(\varepsilon_B-\varepsilon_N)^2}{2}+4t^2\left(\left(\cos\frac{k_y}{2}a\right)^2+\cos\frac{\sqrt{3}k_x}{2}a\,\cos\frac{k_y}{2}a+\frac{1}{4}\right)}$	$a = 1.446$ Å $\varepsilon_B = 4$ eV $\varepsilon_N = 2.1$ eV $t = 1$ eV	Matlab
Matlab [15]	$E = E_0 \pm \gamma_0\sqrt{1+4\cos\left(\frac{\sqrt{3}k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)+4\cos^2\left(\frac{k_y a}{2}\right)}$	$a = 0.246$ nm $E_0 = 0$ eV $\gamma_0 = 2.5 - 3.3$ eV	
Brocks [16]	$E_k = E_p \pm t\sqrt{3+2\cos\left(2\pi k_x\right)+2\cos\left(2\pi k_y\right)+2\cos\left(2\pi\left(k_x+k_y\right)\right)}$	$E_p = 0$ eV $t \approx -3$ eV	-
Moreau [8]	$E = \pm\gamma_n\sqrt{3+f(k)} - \gamma_{nn}f(k)$ $f(k) = 2\cos\left(\sqrt{3}k_x a\right)+4\cos\left(\frac{\sqrt{3}}{2}k_x a\right)\cos\left(\frac{3}{2}k_y a\right)$	$a = 2.46$ Å $\gamma_n = 2.8$ eV $\gamma_{nn} = 0.2\gamma_n$	Matlab
Rozhkov, *et al* [17]	$\varepsilon_k = \pm t\left\lvert 2\cos\left(\sqrt{3}k_y a_0\right)+4\cos\left(\frac{\sqrt{3}}{2}k_y a_0\right)\cos\left(\frac{3}{2}k_x a_0\right)\right\rvert$	$a_0 = 1.42$ Å $t = 2.5 - 3$ eV	-
Adhikary, *et al* [18]	$\varepsilon_k = \pm\gamma_0\sqrt{1+4\cos\left(k_x\frac{3a}{2}\right)\cos\left(k_y\frac{\sqrt{3}a}{2}\right)+4\cos^2\left(k_y\frac{\sqrt{3}a}{2}\right)}$	$\gamma_0 = 2.5 - 3$ eV	Matlab

TABLE II. Rozhkov's formula for graphene's dispersion energy $E(+)$ part.

Cell	Parameter	Formula
A2	lattice constant	= 2.46 Å
B2	hopping parameter	= 2.5 eV
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$2*ABS(2*COS(SQRT(3)*$B6*$A$2)`
	(values in eV)	`+4*COS(SQRT(3)*$B6*$A$2/2)*COS(3*C$5*$A$2/2))`

3. Results

Through the method used, students may easily determine the equations and simulations that match the characteristics of the graphene's dispersion energy. The following is the explanation for each simulation.

Slicing results of Luo (2010), Aydin, *et al* (2011), Muoth (2013), and Adhikary, *et al* (2019) are shown in Figs. 2, 4, 6, and 10. Based on these figures, it can be seen that the slicing at the center of the y, main, and off diagonal axes show a bandgap that is large or not equal to zero. Only the slicing in the center of the x-axis shows a relatively small bandgap. This means that the electrons simply jump along the center of the x-axis.

Fathi (2011) shows the slicing form as shown in Fig. 3. In the figure you can see that the electrons easily jump along the off diagonal. This can be seen from the small bandgap. For slicing in the middle of the x, y axes, and main diagonal the bandgap is quite large. Compared to other equations, Fathi's (2011) four slices show different shapes. In this case, the

a)

C6 =$B$2*ABS(2*COS(SQRT(3)*$B6*$A$2)+4*COS(SQRT(3)*$B6*$A$2/2)* COS(3*C$5*$A$2/2))

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	a	t													
2	2.46	2.5													
3															
4			kx												
5		ky	-2.554	-2.454	-2.354	-2.254	-2.154	-2.054	-1.954	-1.854	-1.754	-1.654	-1.554	-1.454	-1.354
6		-2.554	7.224	6.7756	5.4908	3.5426	1.1932	1.2411	3.4325	5.0861	5.9732	5.9917	5.1218	3.4866	1.3063
7		-2.454	7.4996	7.1675	6.2159	4.7729	3.0328	1.2298	0.3933	1.618	2.2796	2.2888	1.6445	0.4333	1.1815
8		-2.354	7.0932	6.8924	6.3171	5.4446	4.3925	3.3023	2.3209	1.5804	1.1804	1.1748	1.5644	2.2967	3.2731
9		-2.254	5.817	5.7566	5.5835	5.321	5.0044	4.6764	4.3811	4.1583	4.0379	4.0362	4.1534	4.3738	4.6676
10		-2.154	3.6206	3.7033	3.9402	4.2995	4.7328	5.1817	5.5859	5.8908	6.0556	6.0579	5.8974	5.5959	5.1938
11		-2.054	0.6126	0.8347	1.4709	2.4358	3.5994	4.8049	5.8903	6.7092	7.1516	7.1577	6.7269	5.9171	4.8372
12		-1.954	2.9457	2.5943	1.5874	0.0606	1.7806	3.6883	5.4057	6.7016	7.4016	7.4114	6.7296	5.4481	3.7394
13		-1.854	6.6747	6.2099	4.878	2.8582	0.4226	2.101	4.3729	6.0871	7.0131	7.026	6.1241	4.4289	2.1686
14		-1.754	10.133	9.5756	7.9788	5.5575	2.6376	0.3878	3.1114	5.1665	6.2766	6.292	5.2109	3.1786	0.4689
15		-1.654	12.885	12.261	10.471	7.7577	4.4856	1.0952	1.9569	4.26	5.5039	5.5213	4.3097	2.0323	1.0044
16		-1.554	14.573	13.909	12.008	9.1253	5.6488	2.0468	1.196	3.6428	4.9644	4.9829	3.6956	1.276	1.9503
17		-1.454	14.971	14.299	12.372	9.4502	5.9266	2.2757	1.011	3.491	4.8305	4.8492	3.5445	1.0921	2.1779
18		-1.354	14.028	13.377	11.511	8.6823	5.2709	1.7363	1.4457	3.8468	5.1436	5.1617	3.8985	1.5242	1.6416
19		-1.254	11.868	11.268	9.5478	6.9399	3.795	0.5365	2.397	4.6105	5.8061	5.8227	4.6582	2.4694	0.4492
20		-1.154	8.7771	8.2549	6.7586	4.4895	1.7533	1.0818	3.6341	5.56	6.6002	6.6147	5.6016	3.6971	1.1578
21		-1.054	5.1534	4.7328	3.5276	1.7	0.5039	2.7874	4.8431	6.3943	7.2321	7.2438	6.4277	4.8938	2.8486
22		-0.954	1.443	1.143	0.2834	1.0201	2.5919	4.2206	5.6867	6.7931	7.3906	7.399	6.8169	5.7229	4.2642
23		-0.854	1.93	2.0958	2.5709	3.2913	4.1601	5.0602	5.8706	6.4821	6.8123	6.8169	6.4953	5.8906	5.0844
24		-0.754	4.6288	4.6529	4.7221	4.8269	4.9532	5.0842	5.2021	5.291	5.3391	5.3397	5.2929	5.205	5.0877
25		-0.654	6.452	6.3334	5.9934	5.4778	4.8561	4.212	3.632	3.1945	2.9581	2.9548	3.185	3.6177	4.1947
26		-0.554	7.357	7.1009	6.3672	5.2546	3.9129	2.5228	1.2713	0.3269	0.1831	0.1902	0.3066	1.2404	2.4855

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b)

C6 =-$B$2*ABS(2*COS(SQRT(3)*$B6*$A$2)+4*COS(SQRT(3)*$B6*$A$2/2)* COS(3*C$5*$A$2/2))

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	a	t													
2	2.46	2.5													
3															
4			kx												
5		ky	-2.554	-2.454	-2.354	-2.254	-2.154	-2.054	-1.954	-1.854	-1.754	-1.654	-1.554	-1.454	-1.354
6		-2.554	-7.224	-6.776	-5.491	-3.543	-1.193	-1.241	-3.433	-5.086	-5.979	-5.992	-5.122	-3.487	-1.306
7		-2.454	-7.5	-7.167	-6.216	-4.773	-3.033	-1.23	-0.393	-1.618	-2.28	-2.289	-1.644	-0.433	-1.182
8		-2.354	-7.093	-6.892	-6.317	-5.445	-4.392	-3.302	-2.321	-1.58	-1.18	-1.175	-1.564	-2.297	-3.273
9		-2.254	-5.817	-5.757	-5.583	-5.321	-5.004	-4.676	-4.381	-4.158	-4.038	-4.036	-4.153	-4.374	-4.668
10		-2.154	-3.621	-3.703	-3.94	-4.3	-4.733	-5.182	-5.586	-5.891	-6.056	-6.058	-5.897	-5.596	-5.194
11		-2.054	-0.613	-0.835	-1.471	-2.436	-3.599	-4.805	-5.89	-6.709	-7.152	-7.158	-6.727	-5.917	-4.837
12		-1.954	-2.946	-2.594	-1.587	-0.061	-1.781	-3.688	-5.406	-6.702	-7.402	-7.411	-6.73	-5.448	-3.739
13		-1.854	-6.675	-6.21	-4.878	-2.858	-0.423	-2.101	-4.373	-6.087	-7.013	-7.026	-6.124	-4.429	-2.169
14		-1.754	-10.13	-9.576	-7.979	-5.557	-2.638	-0.388	-3.111	-5.167	-6.277	-6.292	-5.211	-3.179	-0.469
15		-1.654	-12.89	-12.26	-10.47	-7.758	-4.486	-1.095	-1.957	-4.26	-5.504	-5.521	-4.31	-2.032	-1.004
16		-1.554	-14.57	-13.91	-12.01	-9.125	-5.649	-2.047	-1.196	-3.643	-4.964	-4.983	-3.696	-1.276	-1.95
17		-1.454	-14.97	-14.3	-12.37	-9.45	-5.927	-2.276	-1.011	-3.491	-4.831	-4.849	-3.544	-1.092	-2.178
18		-1.354	-14.03	-13.38	-11.51	-8.682	-5.271	-1.736	-1.446	-3.847	-5.144	-5.162	-3.899	-1.524	-1.642
19		-1.254	-11.87	-11.27	-9.548	-6.94	-3.795	-0.537	-2.397	-4.61	-5.806	-5.823	-4.658	-2.469	-0.449
20		-1.154	-8.777	-8.255	-6.759	-4.49	-1.753	-1.082	-3.634	-5.56	-6.6	-6.615	-5.602	-3.697	-1.158
21		-1.054	-5.153	-4.733	-3.528	-1.7	-0.504	-2.787	-4.843	-6.394	-7.232	-7.244	-6.428	-4.894	-2.849
22		-0.954	-1.443	-1.143	-0.283	-1.02	-2.592	-4.221	-5.687	-6.793	-7.391	-7.399	-6.817	-5.723	-4.264
23		-0.854	-1.93	-2.096	-2.571	-3.291	-4.16	-5.06	-5.871	-6.482	-6.812	-6.817	-6.495	-5.891	-5.084
24		-0.754	-4.629	-4.653	-4.722	-4.827	-4.953	-5.084	-5.202	-5.291	-5.339	-5.34	-5.293	-5.205	-5.088
25		-0.654	-6.452	-6.333	-5.993	-5.478	-4.856	-4.212	-3.632	-3.194	-2.958	-2.955	-3.185	-3.618	-4.195
26		-0.554	-7.357	-7.101	-6.367	-5.255	-3.913	-2.523	-1.271	-0.327	-0.183	-0.19	-0.307	-1.24	-2.486

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FIGURE 1. Rozhkov's spreadsheet distribution data, a) $E(+)$ and b) $E(-)$ parts.

value of the beta parameter is not specified. If traced using a spreadsheet simulation, it can be seen that the beta parameter does not have much effect on the distance between the valence and conduction bands. So it will still show the simulation intended by Fathi (2011). However, the value of the beta parameter affects the amount of energy dispersion. Because the value of the beta parameter is not specified, in this article we set the value to 1.

Kolb (2012) shows the slicing form as shown in Fig. 5. The four slices obtained show a relatively large bandgap.

TABLE III. Rozhkov's formula for graphene's dispersion energy $E(-)$ part.

Cell	Parameter	Formula
A2	lattice constant	$= 2.46$ Å
B2	hopping parameter	$= 2.5$ eV
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$2*ABS(2*COS(SQRT(3)*$B6*$A$2)`
	(values in eV)	`+4*COS(SQRT(3)*$B6*$A$2/2)*COS(3*C$5*$A$2/2))`

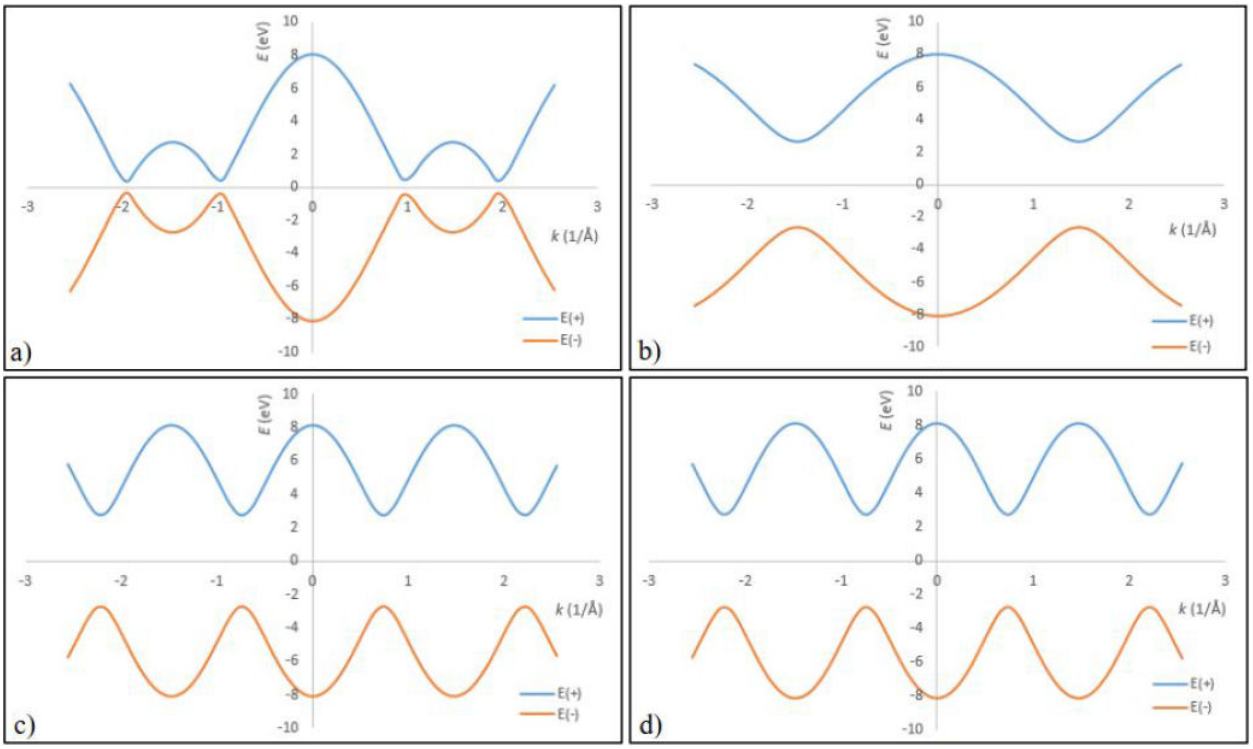

FIGURE 2. Luo's slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

Brocks (2015) shows the slicing form as shown in Fig. 7. Here, the slicing in this equation is different where the valence band is at the top while the conduction band is at the bottom. Slices in the center of the x, y, and off diagonal axes show the same shape and a relatively large bandgap. Only the slicing on the main diagonal shows the bandgap is close to zero. This equation is the only one that has a different slicing between the main and off diagonals.

Moreau (2016) shows the slicing form as shown in Fig. 8. The bandgap is relatively small on the slicing in the middle of the y-axis. Meanwhile, for the slicing in the middle of the x-axis, main, and off diagonal shows a relatively large bandgap.

Rozhkov, *et al* (2016) show a slicing form as shown in Fig. 9. The four slices show that the bandgap is relatively small or close to zero. Electrons easily jump on all four directions, namely the center of the x, y, main, and off diagonal axes. The number of Dirac points is also the largest compared to other equations.

All the slicing that show large bandgap are not in accordance with the characteristics of graphene's dispersion energy. This is because the Dirac point of graphene should have a zero bandgap. In fact these slicing appear to show GO material rather than graphene. Hence, this can be a misconception in understanding graphene's dispersion energy. This misconception can be remedied by referring to the slicing results of Rozhkov, *et al* (2016) as it satisfy the graphene's dispersion energy where all slicing have small or zero bandgaps. Another misconception is produced by the slicing result of Brocks (2015), *i.e.*: switched position of the valance and conduction bands.

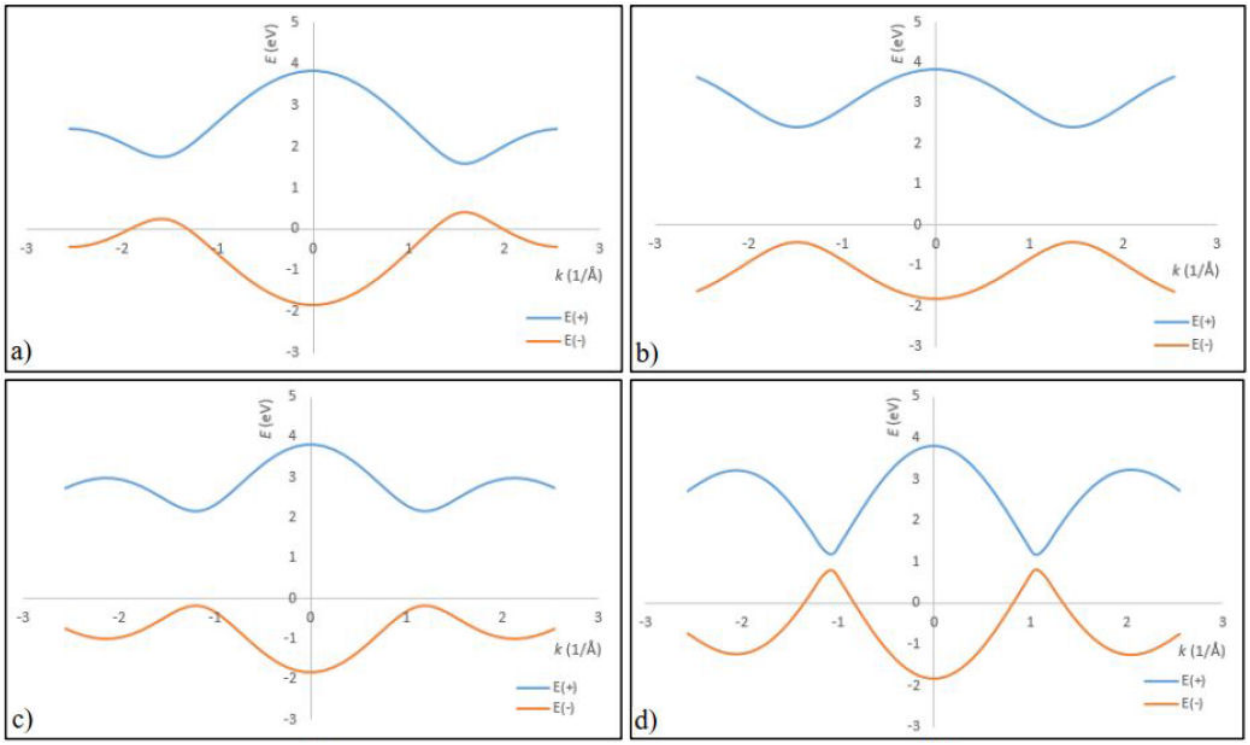

FIGURE 3. Fathi's slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

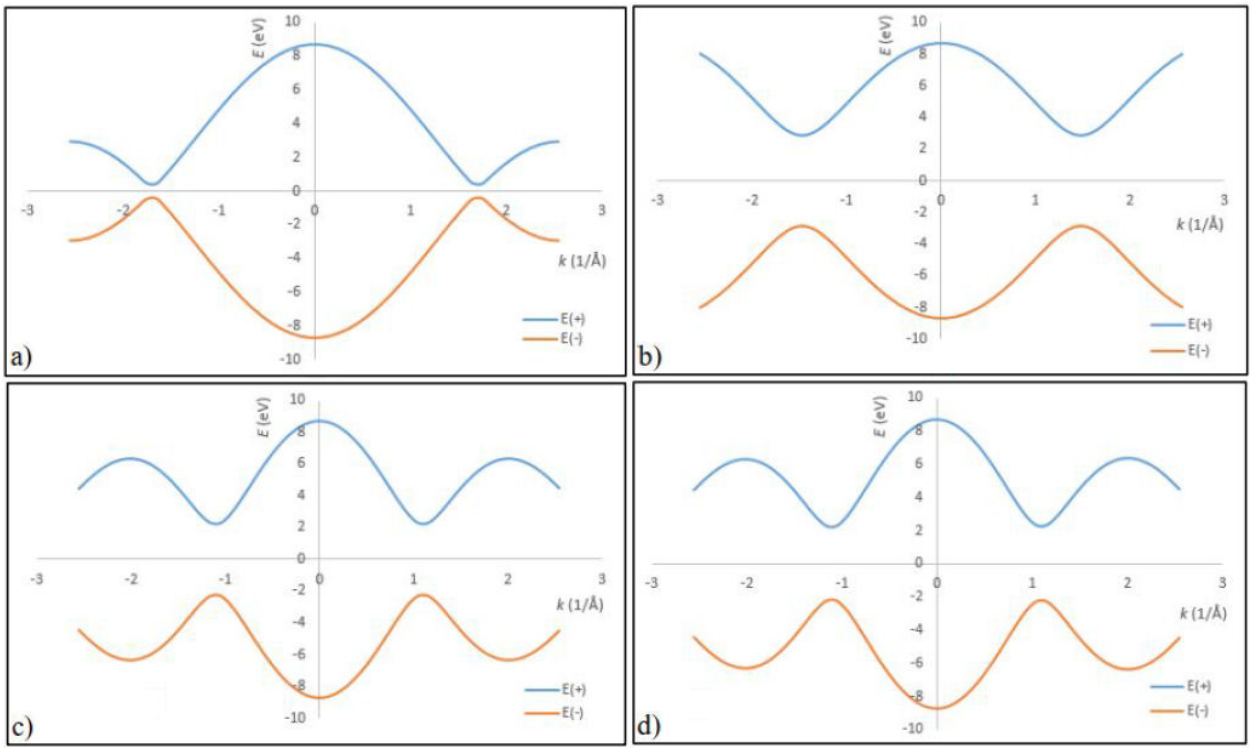

FIGURE 4. Aydin, *et al.'s*, slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

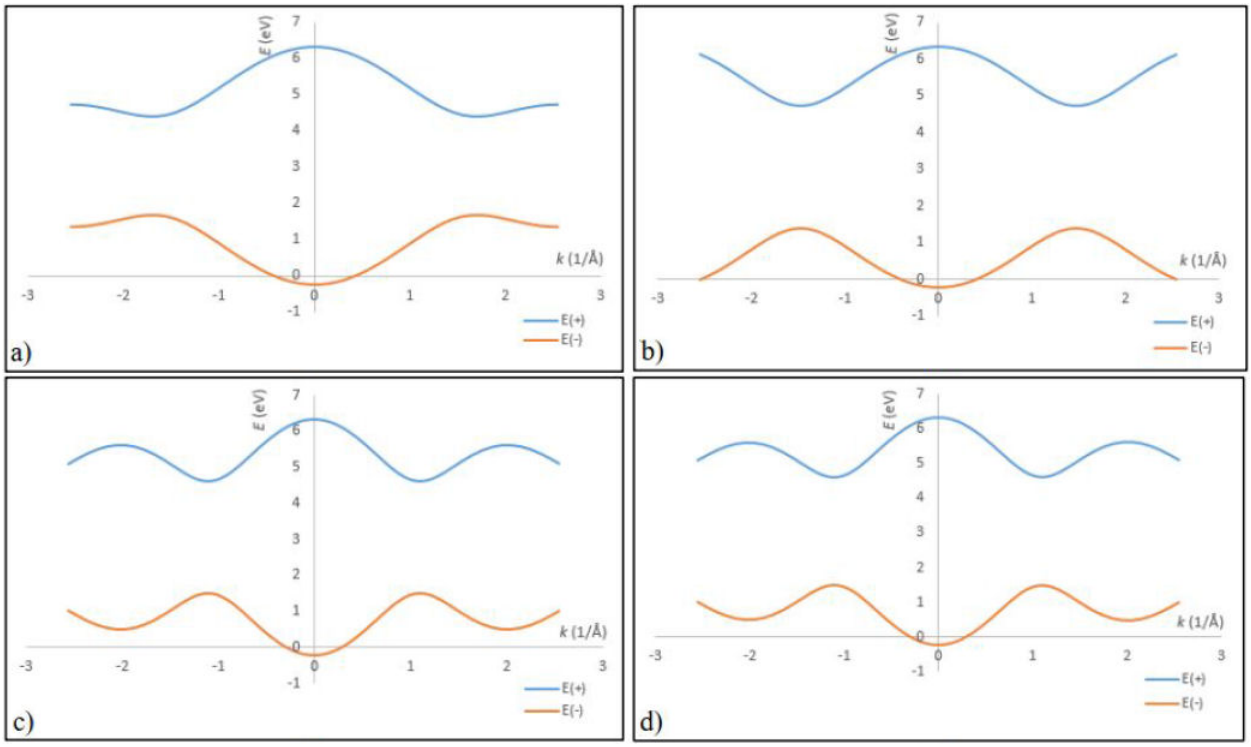

FIGURE 5. Kolb's slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

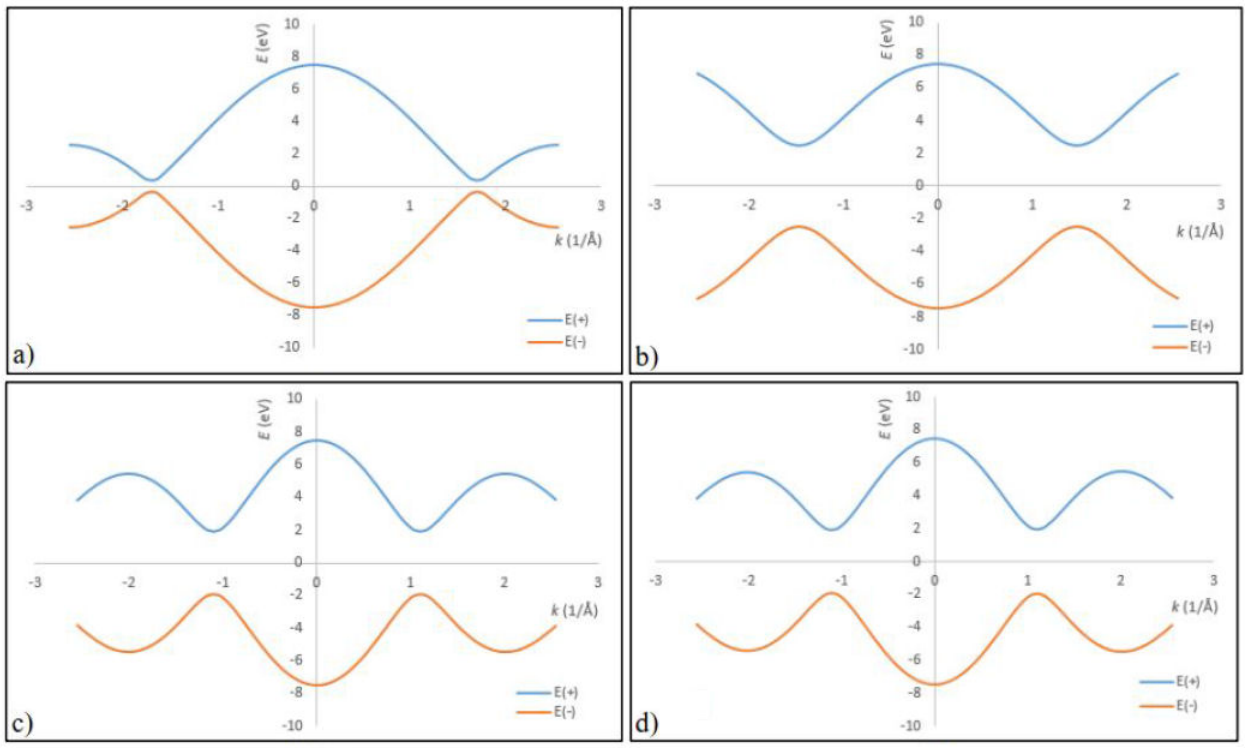

FIGURE 6. Muoth's slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

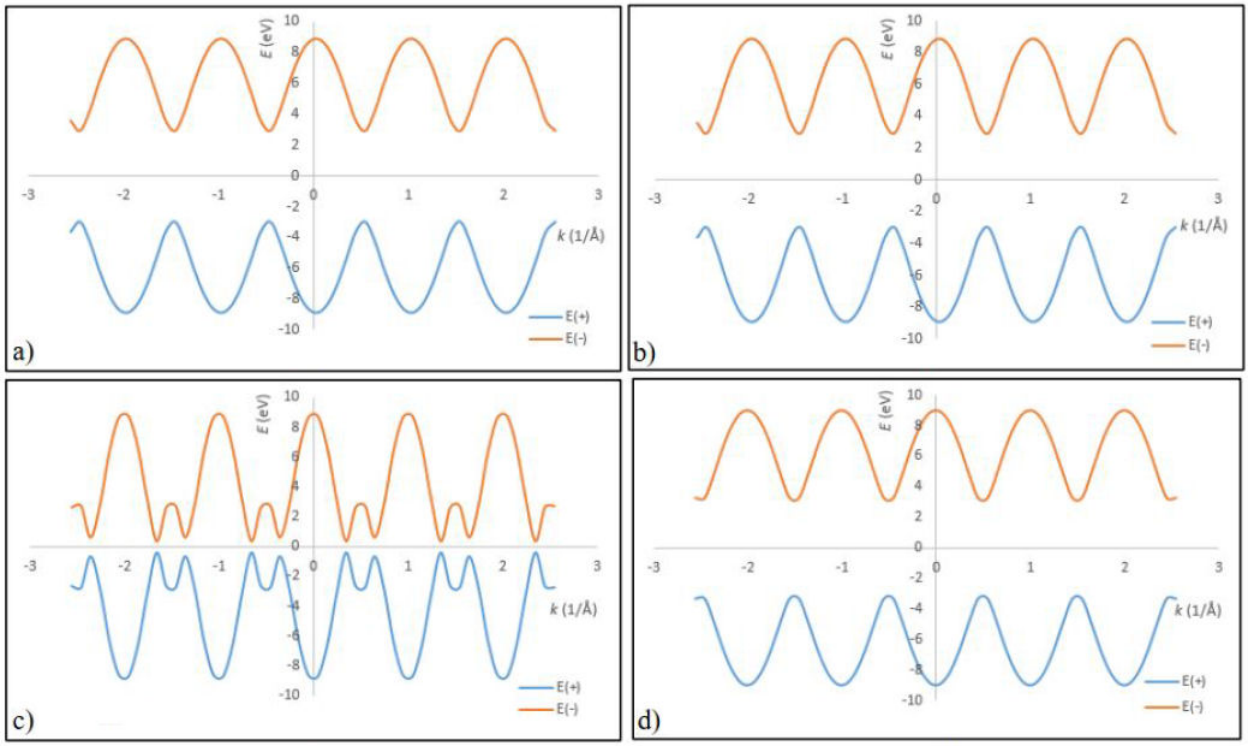

FIGURE 7. Brocks' slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

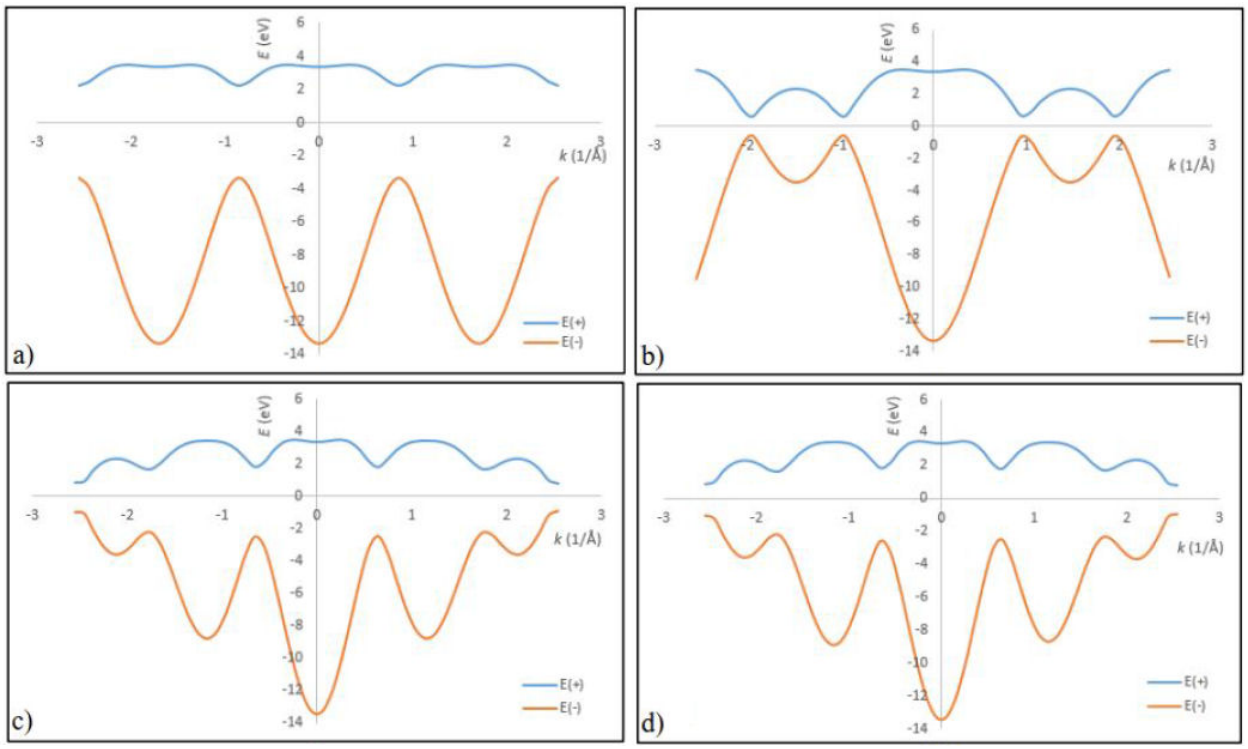

FIGURE 8. Moreau's slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

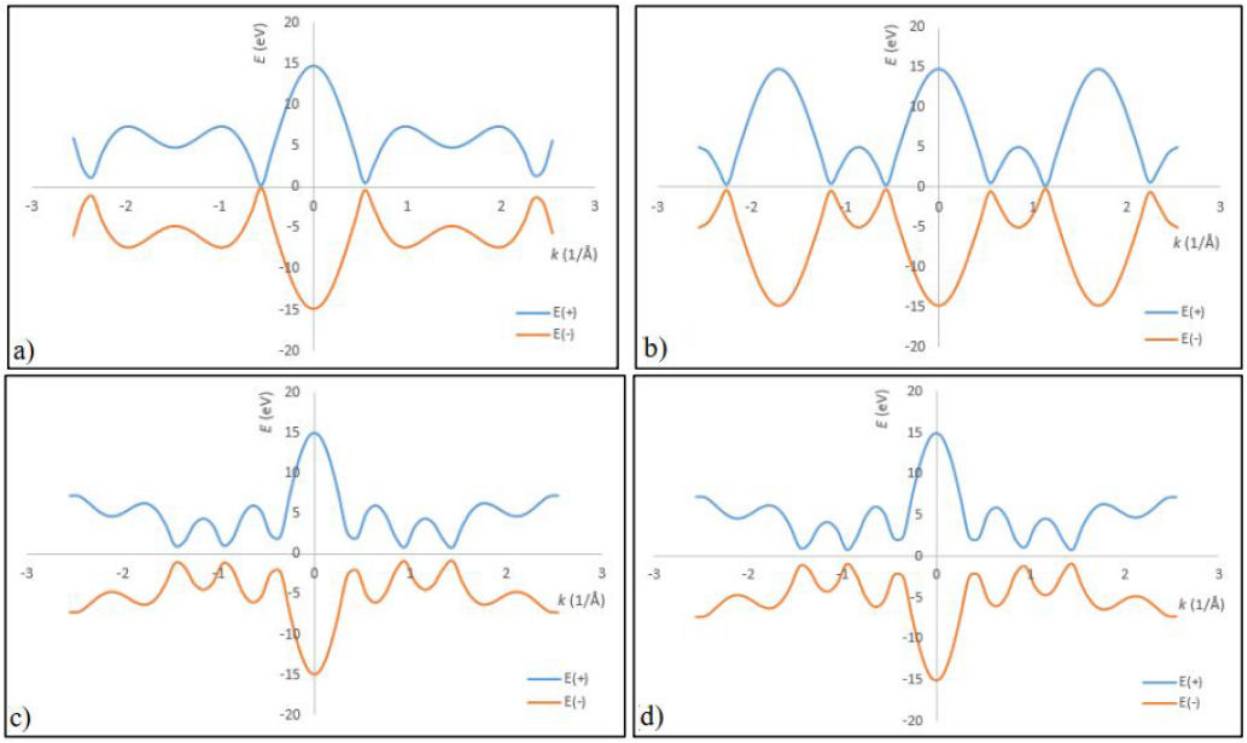

FIGURE 9. Rozhkov, *et al.*'s., slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

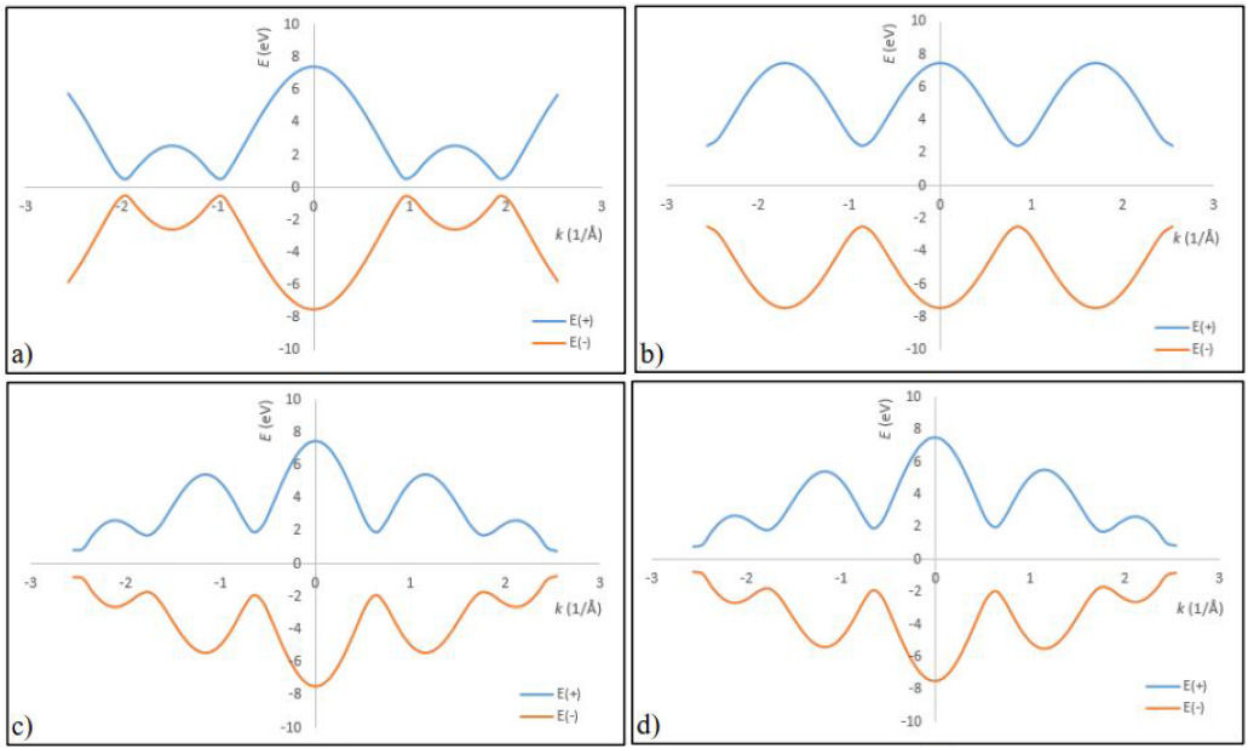

FIGURE 10. Adhikary, *et al.*'s, slicing data, middle a) x and b) y axes, c) main, and d) off diagonals.

4. Conclusion

From this activity, it can be concluded that Rozhkov (2016) has the equations and simulations that best satisfy graphene's dispersion energy. Misconceptions occur in almost all existing equations and simulations. Graphene has Dirac points where the band gap is zero. This means that there is no distance or very small distance between the valence and conduction bands. On average, only one slicing has no or a small bandgap for each equation above. There is one equation where all slicing are far apart, *i.e.*: Kolb (2012). This is certainly not in accordance with the characteristic of graphene's dispersion energy. So it can be concluded that the use of spreadsheets can help students identify the Dirac points in almost all parts of graphene's dispersion energy, especially in the center of the x, y, main, and off diagonal axes.

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