Graphene - Calculation of Specific Surface Area

B. S. Shubha [1], B. M. Praveen [2, 3] and V. Bhat [2, 4,*]

[1] Faculty, Department of Chemistry, Dr. G. Shankar Government Women's First Grade College, Ajjarakad, Udupi-576101, India.
OrcidID: 0000-0003-2104-1410; Email: shubhasanthosh16@gmail.com

[2] Faculty, College of Engineering & Technology, Srinivas University, Mukka-574146. India.

[3] OrcidID: 0000-0003-2895-5952; Email: bm.praveen@yahoo.co.in,

[4] OrcidID: 0000-0002-2246-7870; Email: bhatvasudeva2015@gmail.com

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B. S. Shubha [1], B. M. Praveen [2, 3] and V. Bhat [2, 4,*]
[1] Faculty, Department of Chemistry, Dr. G. Shankar Government Women's First Grade College, Ajjarakad, Udupi-576101, India.
OrcidID: 0000-0003-2104-1410; Email: shubhasanthosh16@gmail.com
[2] Faculty, College of Engineering & Technology, Srinivas University, Mukka-574146. India.
[3] OrcidID: 0000-0003-2895-5952; Email: bm.praveen@yahoo.co.in,
[4] OrcidID: 0000-0002-2246-7870; Email: bhatvasudeva2015@gmail.com

ABSTRACT

Purpose: *Graphene is a wonder material with high potential for application in energy storage supercapacitors owing to its extremely high surface area. Here, a simple and detailed description of calculation of specific surface area of graphene is given in a tutorial like format. From geometric considerations and known values of interatomic distances, it is shown that we can estimate the theoretical surface area of graphene sheets to be ~2630 m^2g^{-1}. Using this approach, teachers will be able to educate their students in various fields where surface area is one of the important factors.*
Approach/Methodology: *Calculation of theoretical maximum specific surface area of graphene using the data like area of a regular hexagon, C-C bond length within the layers in graphene and relative average atomic mass of carbon.*
Findings/Result: *From geometric considerations and known value of interatomic distance in graphite, it is possible to show by calculations that the theoretical surface area of graphene sheets is ~ 2630 m^2g^{-1}.*
Originality/Value: *It is a useful exercise for understanding the simple principles behind such calculations and to appreciate its usefulness in practical applications.*
Paper type: *Review based Analysis.*
Keywords: Graphene, Single layer graphene, Calculation of surface area, Supercapacitor.

1. INTRODUCTION :

Graphenes are sub-units of graphite consisting of one or a few layers of carbon sheets. A graphene consisting of only one such sheet is known as 'single layer graphene' and is abbreviated as SLG. Others, consisting of 2 or more number of layers, are known as 2-layer graphene, 3-layer graphene, etc., and are given a general name: 'few-layer graphene'. Among these, SLG is the best in terms of surface area. When SLG sheets are 3-dimensionally arranged in a zin-zag manner, as in, for example, graphene foam [1, 2] and strutted graphene [3], they would offer their entire surfaces accessible to small ions and molecules. This property has been made use of in electrical energy storage devices, especially, supercapacitors [4-11]. In addition to their (i) high surface area, graphene structures have other desirable beneficial properties such as (ii) high mechanical strength, (iii) high electrical conductivity, (iv) high abundance, (v) low-cost, (vi) ease of synthesis (vii) non-toxicity, (viii) high chemical stability, and (ix) wide working temperature range [10, 11].

2. RELATED WORK :

Table 1 lists typical measured and reported values of some important properties.

Table 1: Some properties of graphene and assembled graphene structures.

S. No.	Property	Measured value	Ref.
1	Specific surface area (experimental)	1,005 $m^2\ g^{-1}$	Wang, X. (2013). [1]

2	Specific electrical capacitance in EDLC configuration	$130 - 250\ F\ g^{-1}$	Wang, X. (2013). [1]
3	Electron mobility	$200{,}000\ \ (cm)^2\ V^{-1}\ s^{-1}$	Morozov, S.V. (2008). [12]
4	Thermal conductivity	$5{,}000\ W\ m^{-1}\ K^{-1}$	Balandin, A.A. (2008). [13]
5	Mechanical strength	Breaking strength: $42\ N\ m^{-1}$ Young's modulus: $\sim 1.0\ TPa$	Lee, C. (2008). [14]

Graphene with high surface area also finds applications in heterogeneous catalysis and membrane science. In all these, high accessible surface area is the main property that makes it ideal for surface-area-dependant applications.
At an introductory level of education on graphene-related materials, calculation of 'theoretical surface area' of single layer graphene (SLG) assemblies is a useful exercise for understanding the simple principles behind such calculations and to appreciate its usefulness in practical applications. In the following, we present a tutorial type explanation of calculation of specific surface area of SLG.

2.1 Graphite And SLG :

Graphite crystals consist of stacks of 2-dimensional graphene sheets (SLGs) held together by weak van der Waal's forces.
The high capacitance of graphene supercapacitors originates from the fact that SLG has a very high surface area. This is due to the 2-dimensional nature of graphene sheets. They are extremely thin nanosheets, being just one-atom thick. Calculation of surface area of SLG, knowing the structure and interatomic distances, gives us an idea about the maximum surface area that can be exploited in supercapacitors and similar applications.

3. OBJECTIVES :

(1) To know about graphite and single layer graphene,
(2) To understand the structural features of graphene.
(3) To calculate theoretical maximum surface area of graphene.

4. METHODOLOGY :

Let us consider a graphene sheet.
Arrangement of carbon atoms in graphene sheets may be represented as in Figure 1.

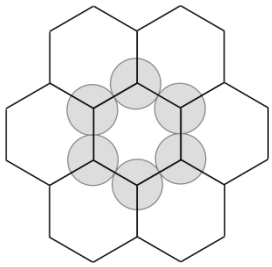

Fig. 1: Diagrammatic representation of a graphene sheet.

In the diagram, all hexagons are regular hexagons, i.e., the edges are of equal lengths. All the edges of all the hexagons represent $C - C$ bonds. All the corners of the hexagons coincide with nuclei of carbon (C) atoms. In the diagram, only six carbon atoms are shown. These atoms are represented as circles. In reality, they are considered to be nearly spherical.

4.1 Surface area:

Let us consider two imaginary planes on two sides of the graphene sheet as shown in Figure 2.

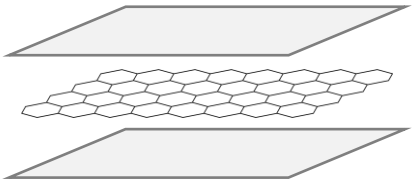

Fig. 2: *A graphene sheet and two planar areas on either side.*

The boundaries of the imaginary planes are equal in lengths to the overall boundaries of the graphene sheet. (Here, we ignore the zig-zag nature of adjacent C- C bonds in graphene sheet's boundary. We take straight line distance between C atoms of corners of the sheet.) The sum of the areas of these two imaginary planes is equal to the surface area of the graphene sheet. (Since the two imaginary planes are of equal size, the sum is equal to twice the area of one imaginary plane.) Thus, for a graphene sheet, the surface area is equal to twice its geometric area.
For example, if the length of the graphene sheet is 10 units and the breadth is 4 units, then the surface area of one side of the sheet is $10 \times 4 = \ 40\ square$ units. So, the total surface area of the sheet, considering both sides, is equal to $2 \times 40 = \ 80\ square$ units.

4.2 Calculation of theoretical maximum specific surface area:

To begin with, we note that 'specific' refers to 'per unit quantity'. Here, 'specific surface area' stands for 'total surface area per unit weight', i.e., 'total surface areas of all SLG sheets present in one gram of graphite'.

- From Math tables [15, 16], we come to know that the area A of a regular hexagon with side a is given by,

$$A = \frac{3\sqrt{3}}{2}\ a^2$$
$$= \frac{3 \times 1.7321}{2}\ a^2$$
$$= 2.5981\ a^2$$

- From references, for example [17], the $C - C$ bond length in graphene is

$$= 0.142\ nm$$
$$= 0.142\ \times 10^{-9}\ m$$
$$= \text{Edge length of the hexagon}$$
$$= a$$

$\therefore$ Area A of the regular hexagon in graphene is

$$= 2.5981\ a^2$$
$$= 2.5981 \times\ (0.142\ \times 10^{-9}\ m)^2$$
$$= 2.5981 \times\ (0.142)^2 \times\ (10^{-9}\ m)^2$$
$$=\ 5.2 \times 10^{-20}\ m^2$$

- In graphene, each C atom is common for 3 hexagons as shown in Figure 1 above.

$\therefore$ Contribution of one C atom of the hexagon to one hexagon is

$$= \frac{1}{3}$$

That is, only one third of a given atom belongs to a given hexagon.
Note: We ignore a very small error in calculation due to considering the carbon atoms at the boundaries (i.e., corners and edges) of the sheet to be same as those inside the sheet. It is reasonable to ignore because, the number of such atoms is small compared to the number of interior carbon atoms in the sheet.

- There are six C atoms at 6 corners of a given hexagon in graphene, as shown in the Figure 1.

$\therefore$ The sum of contribution of all six C atoms of a given hexagon to that hexagon is

$$=\ 6 \times \frac{1}{3}$$
$$= 2$$

Thus, there are effectively two full C atoms per hexagon.

- So, area occupied by these two C atoms = the area of the hexagon.

∴ Area per single C atom is half of the area of the hexagon

$= \frac{A}{2}$

- We know that a two-dimensional sheet has two surfaces.

So, surface area per C atom is twice the above value, i.e.,

$= \frac{A}{2} \times 2$

$= A$

$= 5.2 \times 10^{-20}\ m^2$, as calculated above.

- From tables, the relative average atomic mass (i.e., atomic weight) of element carbon is

$= 12.011$

≈ 12

∴ Mass of a C atom is $12\ amu$

From tables,

$1\ amu = 1.6605 \times 10^{-27}\ kg$

∴ Mass of a C atom is

$= 12 \times 1.6605 \times 10^{-27}\ kg$

$= 1.9926 \times 10^{-26}\ kg$:

- Specific surface area (i.e., area per unit mass) of graphene

$$= \frac{Surface\ \ area\ \ \ offered\ \ \ by\ a\ single\ C\ atom\ in\ graphene}{Mass\ of\ a\ single\ C\ atom}$$

$$= \frac{5.2 \times 10^{-20}\ m^2}{1.9926 \times 10^{-26}\ kg}$$

$$= \frac{5.2}{1.9926} \times 10^{-20+26}\ \frac{m^2}{kg}$$

$= 2.629 \times 10^6\ m^2\ (kg)^{-1}$.

The unit, $m^2\ (kg)^{-1}$, is the SI unit. A useful practical unit, commonly used in the literature, is $m^2\ g^{-1}$. (The required conversion factor already appears as k in the SI unit.)

4.3 Expressing the specific surface area of graphene in units of $m^2\ g^{-1}$:

In the above value, we put 10^3 in the place of k, since k stands for kilo and $kilo = 1000$.

Specific surface area of graphene, in units of $m^2\ g^{-1}$,

$= 2.629 \times 10^6\ m^2\ (10^3\ g)^{-1}$

$= 2.629 \times 10^6\ m^2 \times (10^3)^{-1} \times (g)^{-1}$

$= 2.629 \times 10^6\ m^2 \times 10^{-3} \times g^{-1}$

$= 2.629 \times 10^{(6-3)}\ m^2\ g^{-1}$

$= 2.629 \times 10^3\ m^2\ g^{-1}$

$\approx 2{,}630\ m^2\ g^{-1}$

5. COMPARISON :

For comparison, the area of a $50\ m \times 50\ m$ field is $= 2{,}500\ m^2$. The theoretical maximum surface area of 1 gram of graphene is larger than the area of this field.

6. ABCD ANALYSIS, ACCORDING TO AITHAL ET. AL. (2019) [18] :

When the content of this paper and the method adapted to present it are viewed under ABCD (advantages, benefits, constraints and disadvantages) analysis framework, proposed by Aithal et. al. [18], we can observe the following:

6.1 Advantages of calculating theoretical surface are of graphene:

This method can be applied to calculate surface area of any material with crystallogrphically well defined atomic positions.

6.2 Benefits of calculating theoretical surface are of graphene:

Both teachers and students will be benefited.

6.3 Constraints of calculating theoretical surface are of graphene:

Though a two-dimensional representation of atoms, as shown in Figure 1 is perceivable, it would be more impressive if it were presented with a 3D view. Present technology needs more effort to give such a presentation in a simple manner through publications in electronic media.

6.4 Disadvantages:

There are no disadvantages.

6. CONCLUSION :

A tutorial type presentation of calculation of theoretical surface area of graphene sheets, ~ 2,630 $m^2\ g^{-1}$, is given. It is hoped that teachers will find this useful for educating their students in different fields at appropriate levels of education. In a typical class-room session, it is recommended that teachers will provide to their students five essential pieces of information namely, (1) the hexagonal structure of graphene, (2) the mathematical equation for area of a regular hexagon of side a, $Area = \left(\frac{3\sqrt{3}}{2}\right) a^2$, (3) the C- C bond length, $0.142 \times 10^{-9}\ m$, within the layers in graphene, (4) the relative average atomic mass, 12.0, of carbon and (5) the conversion factor, $1\ amu = 1.66 \times 10^{-27}\ kg$, as data.

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