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LITERATURE REVIEW OF THEORETICAL STUDIES OF PHOSPHORENE AND GRAPHENE AS GAS SENSOR FOR CARBON DIOXIDE[1]

REVISÃO BIBLIOGRÁFICA DOS ESTUDOS TEÓRICOS SOBRE O FOSFORENO E O GRAFENO COMO SENSOR PARA DIÓXIDO DE CARBONO

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ABSTRACT

Two-dimensional nanomaterials, such as graphene and phosphorene, has been attracting researchers' interest, due to their possible applications. One of their applications is as gas sensors. Carbon dioxide is a gas, which needs to be monitored because it is one of the responsible for the greenhouse effect and for the changes in temperature. Therefore, the aim of this paper is to organize a literature review of the theoretical articles that use the Density Functional Theory to study graphene and phosphorene as carbon dioxide sensors. Analyzing the adsorption energies of the papers reviewed it is concluded that graphene and phosphorene are more promising sensors for carbon dioxide when this molecule is adsorbed on the graphene edged or when it is adsorbed on doped phosphorene. This literature review opens new perspectives for experimental studies.

Keywords: adsorption, nanomaterial, Density Functional Theory.

RESUMO

Os nanomateriais bidimensionais, como o grafeno e o fosforeno, tem atraído interessante da comunidade científica devido as suas possíveis aplicações. Uma das aplicações destes nanomateriais é em sensores de gases. O dióxido de carbono é um gás que necessita ser monitorado devido ao fato de ser um dos responsáveis pelo efeito estufa e pelas mudanças de temperaturas. Esta revisão de literatura abre perspectivas para estudos experimentais e tem como objetivo realizar um levantamento bibliográfico dos artigos teóricos que utilizam a Teoria do Funcional da Densidade para estudar o grafeno e o fosforeno como sensores do dióxido de carbono. Analisando as energias de adsorção dos estudos considerados, é possível observar que o grafeno e o fosforeno são sensores promissores para o dióxido de carbono, quando a molécula é adsorvida na borda do grafeno ou quando é adsorvida no fosforeno dopado.

Palavras-chaves: *adsorção, nanomateriais, Teoria do Funcional da Densidade.*

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INTRODUCTION

Two-dimensional materials (2D), in which electrons are free in two directions and confined in one and have a large surface area, have interesting physical properties that allows its application in several areas (GAN; HU, 2011). The unceasing interest in 2D nanomaterials leads researchers to study different applications of these materials.

Among the most studied 2D nanomaterials is highlighted the graphene, carbon allotrope, which has attracted the attention of researchers because of its electronic and structural characteristics that allow its application in several areas, such as electronics, mainly in field-effect transistors, and medicine, including drug delivery, cancer therapies and biosensing (ABERGEL et al., 2010; FENG; LIU, 2011; REDDY et al., 2011). Another important 2D nanomaterial is the phosphorene, phosphorus allotrope, which has properties that allow it to be considered as the 2D material of the next generation, with promising primarily applications on electronics, including sensors and transistors (LIU et al., 2014; ZHANG et al., 2014).

Sensors are largely used in the control of emission of automotive gases, gases responsible for global warming and greenhouse gases; also, in detection in leakage of gases in industries (MITCHELL, 1989; TWIGG, 2007). Nanotechnology applied to sensors enables high-performance devices much faster, what can operate at low temperatures, resists to thermal shock and avoids the use of expensive catalysts, which can lower its cost when compared to macroscale devices (SHARMA; MADOU, 2012).

Carbon dioxide (CO_2) is one of the gases responsible for climate changes. The global emission of this gas is a consequence of fossil fuels combustion, which increased by an average of 2.5% per year in the last decade. Two-thirds of CO_2 emission consists in an increasing of approximately 2°C in the temperature, which will be deplete in 30 years (FRIEDLINGSTEIN et al., 2014). Proposals to reduce emission of gases responsible for the greenhouse have been continuously presented. The Kyoto protocol, for example, effectively implemented in 1997, has presented the "carbon credits", in which each ton of CO_2 that is not released into the atmosphere guarantee one credit for the company (GRUBB; VROLIJK; BRACK, 1997).

Experimental studies about phosphorene as sensor need to be developed; however, there is in literature experimental studies of graphene as gas sensor for CO_2 (HAFIZ et al., 2014; LIANG et al., 2011; YOON et al., 2011). Yoon et al. (2011) report high performance of graphene for the detection of carbon dioxide, which unlike other sensors, can operate under different temperatures. Yoon observed a linear increased on conductance in cases, which CO_2 concentration increases from 10 to 100 ppm; therefore, this sensor presented high sensitivity, fast response in short time and low power consumption.

In literature, theoretical studies of graphene and phosphorene as CO_2 sensors are found. Therefore, this paper aims to perform a literature review of theoretical studies on graphene and phosphorene as CO_2 sensors, evaluating the adsorption of this molecule in these 2D nanostructures. With this

study, it will be possible to highlight which nanostructures under study has the greatest potential to be applied as CO_2 sensor.

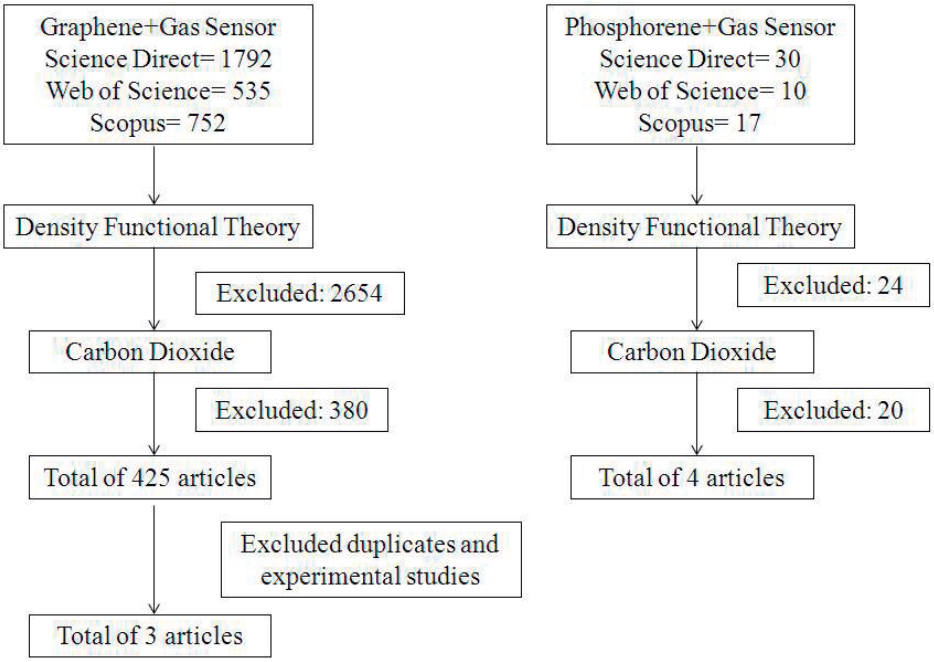
MATERIAL AND METHODS

In order to produce this study, a bibliographical research was developed to explore theoretical studies on the use of graphene and phosphorene as CO_2 sensor. Only studies using computational simulations based on the DFT (HOHENBERG; KOHN, 1964) were considered. This theory is based on quantum mechanics and uses electronic density to obtain all information about the system.

The search for publications was executed on the following databases: Web of Science, Scopus and Science Direct, from 2014 until 2017. The year of 2014 was chosen due to the fact that in this year, studies on phosphorene started. No language restrictions were used. Only articles published in scientific journals were considered, excluding publications in events.

Two researches were performed separately, as presented in the flowchart in figure 1. Firstly, theoretical scientific articles about graphene as CO_2 sensor were searched, using the words graphene, gas sensor, Density Functional Theory and Carbon Dioxide as descriptors. Later, theoretical scientific articles of phosphorene as CO_2 sensor were searched, the words used as descriptors were: phosphorene, gas sensor, Density Functional Theory and Carbon Dioxide.

Figure 1 - Flowchart on words used as descriptors and the method of exclusion.



Source: author's construction.

After the exclusion criteria, seven scientific papers were considered. Three on graphene as CO_2 sensor and four on phosphorene. The computational code used to perform the simulations and

gases under study were observed. Also, it was observed the exchange-correlation term used, or Local Density Approximation (LDA), or generalized gradient approximation (GGA), or Becke, three-parameter, Lee-Yang-Parr (B3LYP) approximation. In addition, the adsorption/interaction energies and conclusions of the authors on the interaction between CO_2 and nanostructures were highlighted.

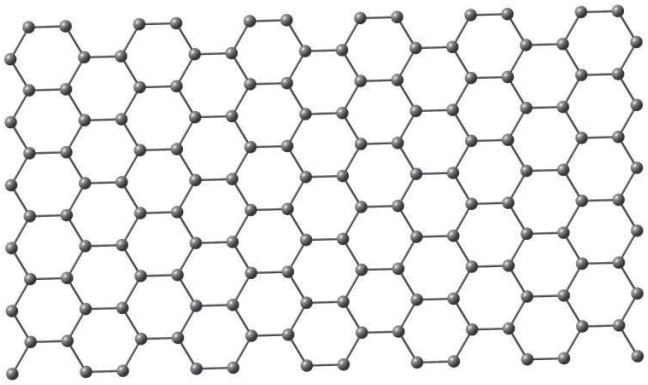
RESULTS AND DISCUSSION

First, to introduce the properties of graphene and phosphorene it was used other papers, beyond the papers considered on the literature review. Afterwards, the results of the scientific articles considered are presented.

CHARACTERISTICS OF GRAPHENE AND PHOSPHORENE

Discovered by Novoselov et al. (2004) graphene is a two-dimensional material built only of carbon atoms, one can see its structure in figure 2. Graphene is the most studied carbon allotropes and can be understood as a monolayer, or sheet, composed of carbon atoms.

Figure 2 - Geometric representation of graphene. Gray spheres represent carbon atoms and gray bonds represent the bonds between these atoms.



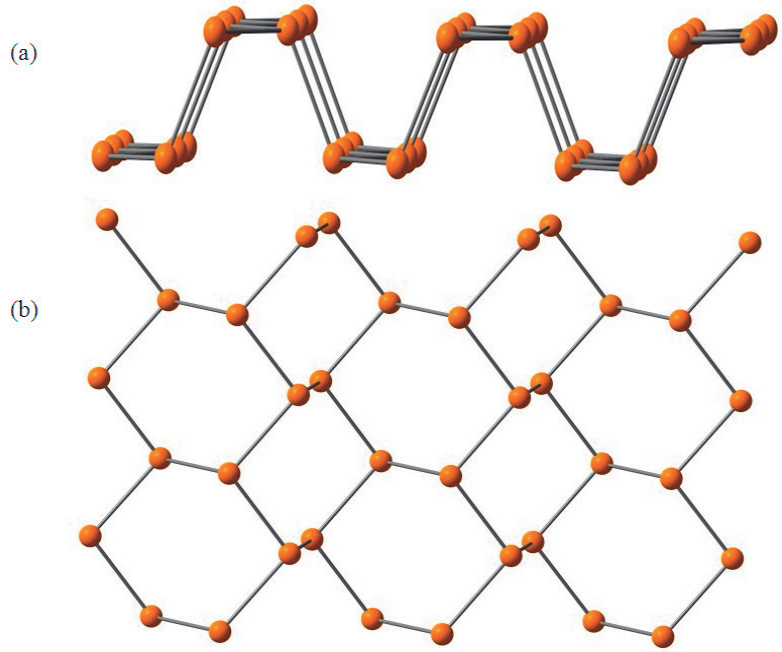
Source: author's construction.

Graphene presents good flexibility in different pressure conditions with a Young's modulus of 1.0 TPa (1000 GPa) (TAN et al., 2013). The electron mobility for graphene is extremely high at room temperature of about 1500 cm^2/ (V.s) (HWANG; ADAM; SARMA, 2007). In addition, graphene presents a semiconductor characteristic with zero energy gap (SAITO et al., 1992) and maximum thermal conductivity of 5000 W/(m.K) (LEE et al., 2008). Its specific area is 2360 m^2g^{-1}, which makes it attractive for many applications, such as, field effect transistors, conductive and transparent films, sensors, clean energy devices and polymer nanocomposites (ZHU et al., 2010). It can be

obtained by chemical exfoliation, mechanical exfoliation and chemical vapor deposition (ZHU et al., 2010; SOLDANO; MAHMOOD; DUJARDIN, 2010). The most used method is mechanical exfoliation because it has low cost and can be produced in large scale (YI; SHEN, 2015).

Similar to carbon, phosphorus present allotropes, as phosphorene. Discovered in 1914, by Bridgman (BRIDGMAN, 1914), this nanostructure is a monolayer of phosphorus. Figure 3 presents its geometric representation, in which is observed that phosphorene present puckered structure.

Figure 3 - Geometric representation of phosphorene (a) side view and (b) top view.
Orange spheres represent P atoms and gray bonds represent the bonds between these atoms.



Source: author's construction.

The Young's modulus of phosphorene is 166 GPa along the zigzag direction and 44 GPa along the armchair direction, which guarantees it excellent flexibility (WEI; PENG, 2014). It is a material with a direct semiconductor characteristic with a gap of approximately 1.5 eV (LI et al., 2014) and has electron mobility of 1000 cm^2 / (V·s). It presents thermal conductivity of 36 W / (m ·K) in the armchair direction (JAIN; MCGAUGHEY, 2015). These properties allow numerous applications, highlighting in various branches of electronics, such as: batteries, transistors, photovoltaic cells, optical-electronics and sensors, being widely studied as sensors for gases (BAGHERI; MANSOURI; AGHAIE, 2016, LIU et al., 2014). This nanomaterial can be obtained through mechanical cleavage, liquid exfoliation or chemical vapor deposition (KOU; CHEN; SMITH, 2015). The most studied method of extraction is the liquid exfoliation, which allows the production of phosphorene on a large scale (BRENT et al., 2014).

Table 1 summarizes the characteristics of graphene and phosphorene, including mechanical, thermal and electrical properties of those nanomaterials.

Table 1 - Properties of graphene and black phosphorene.

Properties	Graphene	Phosphorene
Young's Module (GPa)	1000 (TAN et al., 2013)	166 - 44 (WEI; PENG, 2014)
Electron Mobility ($cm^2/(V \cdot s)$)	1500 (HWANG; ADAM; SARMA, 2007)	1000 (JAIN; MCGAUGHEY, 2015)
Gap (eV)	0 (SAITO et al., 1992)	1 - 1.5 (LI et al., 2014)
Thermal conductivity (W/(m·K))	5000 (LEE et al., 2008)	36 (110) (JAIN; MCGAUGHEY, 2015)

GRAPHENE AND PHOSPHORENE AS CO_2 SENSOR

Table 2 shows the summary of the papers analyzed, nanostructures studied, which atom was used to doped the structure, which gases are under study, what computational code was used, which binding/adsorption energies (in module) were obtained and respective references. All analyzed studies used DFT to study interactions between CO_2 and other gases used with graphene or phosphorene.

Table 2 - Table with studies of phosphorene and graphene as CO_2 sensors, with bindings/adsorption energies (E_b). *Values are considered in module.

Nanostructure	Doped with	Gas	Computacional Code	Term	E_b/CO_2* (eV)	Reference
Graphene	Al	CO, CO_2 and H_2O	Gaussian 03	B3LYP	Pristine 0.04 Al 1.06	Rad e Foukolaei (2015)
Graphene	Pristine	CO_2	GAMESS	B3LYP	Pristine 0.04 Armchair 0.37 Zigzag 3.89	Noei (2016)
Graphene	B, N, and B-N	CO, CO_2, NO and NO_2	VASP	GGA	Pristine 0.11 B and N 0.12 B-N 0.25	Choudhuri et al. (2015)
Phosphorene	Pristine	CO, CO_2, NH_3, NO, and NO_2	VASP	LDA	0.41	Kou, Frauenheim e Chen (2014)
Phosphorene	Vacancy	H_2, N_2, CO, CO_2, H_2O and CH_4	Quantum ESPRESSO	GGA	0.22	Zhang et al. (2016)
Phosphorene	Ca	CH_4, CO_2, H_2 and NH_3	VASP	GGA	Pristine 0.15 Decorated 0.37	Lalitha, Nataraj e Lakshmipathi (2016)
Phosphorene	Pristine	CH_4, CO_2	GCMC	B3LYP	0.27	Zhang et al. (2017)

Rad and Foukolaei (2015) studied the interaction between pure and Al-doped graphene with gaseous molecules of CO, CO_2 and H_2O. Doping is considered when a C atom is replaced by an atom and Al. This study evaluated electronic properties, adsorption energy and charge transfer using B3LYP and Gaussian 03 computational code. The adsorption energy obtained for the most stable interaction between pure graphene and CO_2 was 3.71 kJ. mol^{-1} (0.04 eV) and for the most stable in-

teractions between Al-doped graphene and CO_2 was 102.6 kJ.mol^{-1} (1.06 eV). The adsorption of the molecule with pure graphene is considered physical adsorption due to its low energy value. While the adsorption on graphene doped with Al is chemical, due to the high binding energy value. These results indicate Al-doped graphene is a more promising CO_2 sensor than pure graphene.

The configurations considered in the study of CO_2 adsorption at the center and at the edges of graphene performed with B3LYP and General Atomic and Molecular Electronic Structure System (GAMESS) code (NOEI, 2016). Adsorption at the center of graphene sheet has adsorption energy of 1.1 kJ/mol (0.04 eV), and the adsorption energy at armchair edge was 8.5 kJ/ mol (0.37 eV), both are considered as a physical adsorption. Adsorption of CO_2 at zigzag edge of graphene presented adsorption energy of 89.5 kJ /mol (3.89 eV), characterizing the adsorption as chemical. These results indicate an effective adsorption of CO_2 at zigzag edges.

In the study developed by Choudhuri et al. (2015) adsorption of CO, CO_2, NO and NO_2 on pure and doped graphene with B, N and B-N was analyzed using GGA and Vienna ab initio simulation package (VASP) code. Doped graphene interacts strongly with gaseous molecules; B-N doped graphene was more efficient than B-, N- and pristine-graphene, since it changed the electronic properties of the system after the interaction. The adsorption energy for the interaction between pure graphene and CO_2 was 0.11 eV, B-doped graphene and CO_2 was 0.12 eV, N-doped graphene with CO_2 was 0.12 eV and for B-N doped graphene it was 0.25 eV. Therefore, it was concluded that B-N doping increases adsorption and selectivity of graphene as CO_2 sensor.

To study hydrogen separation of phosphorene with vacancy, the selectivity and permeability of H_2 compared to N_2, CO, CO_2, H_2O and CH_4 was evaluated (ZHANG et al., 2016). All gaseous molecules under study were positioned near the vacancy created in phosphorene and all calculations used GGA and Quantum ESPRESSO code. Researchers found adsorption energy for all gases ranging from 0.04 eV to 0.36 eV. The adsorption energy between phosphorene with vacancy and CO_2 molecule was 0.22 eV, weak interaction, caused by Van der Waals force.

Lalitha et al. (2016) used GGA and the VASP code to study the adsorption of CH_4, CO_2, H_2 and NH_3 on pure, doped and decorated Ca phosphorene. Doping is considered when a P atom is replaced by an atom and Ca, while in the decorated case, is considered when a Ca atom is positioned next to the phosphorene sheet. In the interaction with pure phosphorene the binding energy for the CO_2 found is 0.147 eV. The binding energy for the interaction between CO_2 and phosphorene decorated with Ca was 0.346 eV, a characteristic value for weak interaction. The authors mention the binding energy of the interaction between CO_2 and Ca-doped phosphorene is also negative, but do not include the value. Kou et al. (2014) evaluated the adsorption of the CO, CO_2, NH_3, NO, and NO_2 molecules on the surface of the pure phosphorene. The results indicated that the adsorption energy of the interaction 0.41 eV. Both Latitha (2016) and Kou e Frauenheim (2014) indicated phosphorene as a promising material as a CO_2 sensor.

The study of the adsorption of CO_2 in the phosphorene, and its separation of natural gas was realized with B3LYP and with the Grand Canonical Monte Carlo (GCMC) computational code (ZHANG et al., 2017). The results indicate that CO_2 can be easily adsorbed on the surface of the phosphorene, with the adsorption energy of the interaction of 0.27 eV. The difference in adsorption energy between CO_2 and CH_4 adsorbed on the surface of phosphorene is 0.16 eV, indicating that it is possible to separate CO_2 gas from CO_2 / CH_4 using phosphorene. It was concluded that this nanomaterial is a promising candidate for natural gas purification and gas adsorption.

CONCLUSION

In this literature review, a brief summary of the properties of 2D nanomaterials, graphene and phosphorene for the detection of CO_2 gas was presented. Seven papers were analyzed, three of them used the VASP computational code to perform the simulations and three studied the pure nanostructures. One scientific paper studied the adsorption of CO_2 in the nanostructures, others analyzed in the same study the adsorption of other gas molecules.

Observing the results obtained in the articles considered, for the CO_2 and graphene interaction the work developed by Noe1 (2016), showed an adsorption energy of 0.04 eV when the gas is adsorbed at the center of the graphene sheet (physical adsorption) and 3.89 eV in CO_2 adsorption at the zigzag edge of graphene (chemical adsorption). Among all the publications considered, this one, with adsorption by the edge, presented greater efficiency for a possible use of this nanomaterial like gas sensor.

The study developed by Kou, Frauenheim and Chen (2014) indicated that pure phosphorene showed promise for use as CO_2 sensor, because the energy of adsorption energy found was 0.41 eV. Another study that presented promising results was the one developed by Lalitha et al. (2016) in which they obtained adsorption energies of 0.35 eV for the phosphorene decorated with Ca, indicating that the doping of the phosphorene with Ca corroborated in the adsorption of the gas on the surface of this nanomaterial. It is believed that the difference between the values occurred due to the use of different terms of exchange and correlation, since the term used by Kou (2014) tends to overestimate the binding energy values.

It is important to highlight the edge and doping effect. It is concluded that the edge effect and the doping of 2D nanomaterials can make the materials more promising for applications in gas sensors, mainly as CO_2 sensors. Therefore, it is suggested to carry out the study on the adsorption of CO_2 at the edges of phosphorene. In addition, this literature review sought to encourage future experimental studies, mainly on phosphorene as CO_2 sensors, since experimental studies with graphene already exist in the literature. Theoretical and experimental studies on 2D nanostructures as gas sensors aim to make these devices faster, more efficient and low energy cost.

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