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INTERACTION OF THE WAVE PACKET AND GRAPHENE SHEET AND CRITICAL TEMPERATURE OF HYDROGEN STORAGE

D. Malivuk[1,*], *S. Nježić*[2], *S. Lekić*[1], *Z. Rajilić*[1]

[1] University of Banja Luka, Faculty of Science and Mathematics, B&H
Mladena Stojanovića 2, 78000 Banja Luka
[2] University of Banja Luka, Faculty of Medicine, Save Mrkalja 14, 78 000 Banja Luka, B&H

Abstract: Concerning to their industrial application, testing of the performances of nanomaterials is very important . Research of graphene characteristics is important for the storage of hydrogen. In this paper the interaction of the wave packet was simulated with one graphene sheet and the results were studied. Temperature T_f was calculated, whereby, for $T \leq T_f$, the graphene sheet can significantly affect the movement of a wave packet, while the movement of the wave packet is not significantly affected for $T > T_f$. We analyzed the functional dependence of temperature T_f on the sheet shapes and sizes. The question under which conditions the temperature T_f is suitable for significant hydrogen storage is a very interesting issue. Approximate quantum Newton's equation was used for calculation. Guisbiers and Buchaillot discussed the dependence of the size and shape of nanostructures (graphene sheet) and characteristic temperatures of transition. The results obtained by computer experiments partly agree with the equation proposed by Guisbiers and Buchaillot. The computations were done using Runge-Kutta-Fehlberg method and partly agree with equation. Guisbiers and Buchaillot discussed the dependence of nanostructure size and shape (graphene sheet) and characteristic temperature (phase) transition, suggesting a universal equation, in which case our results can be fitted with a curve of this form for certain temperature intervals.

Keywords: graphene, hydrogen storage, Newton's quantum equation.

1. INTRODUCTION

Hydrogen storage on the nanostructure level is considered to be one of the most important factors for improving the performance and efficiency of the fuel cells [1]. The recently produced mono and double layer sheets of graphite – graphene have some exquisite properties, giving rise to a hope that with these nano-objects the expected storage capacity can be reached. Graphene is a single atomic plane of graphite, which, and this is essential, is sufficiently isolated from its environment to be considered free-standing [2].

Research of graphene has developed rapidly over the last few years. Several papers appear every day, and, if the bibliometrics predictions are to be trusted, we will continue to see a rapid increase in the amount of literature on graphene over the next few years.

A safe and efficient storage of hydrogen is a crucial step towards its use in the future as an energy vector. Adsorption of hydrogen on graphene (G) can take place in different ways: (i) by physisorption of molecular hydrogen, (ii) by physisorption of atomic hydrogen, (iii) by chemisorption of atomic hydrogen, (iv) by chemisorptions of small clusters of atomic hydrogen. These scenarios exhibit different adsorption/desorption energies, optimum geometrical configurations and diffusion barriers.

Hydrogen chemisorption on graphene and graphite surfaces has been extensively studied both experimentally and theoretically.

Guisbiers and Buchaillot discussed the dependence of the size and shape of nanostructures (graphene sheet) and characteristic temperatures of transition [3].

Conditions for hydrogen storage can be improved if impurities are added to graphene , that is to say, if there is another adsorbed element on the surface of the graphene sheet [5].

[*] Corresponding author: draganamalivuk@yahoo.com

2. TRAJECTORIES OF WAVE PACKAGE CENTRE

In this paper the interaction of the wave packet with one graphene sheet was simulated. Temperature T_f was calculated, whereby, for $T \leq T_f$, graphene sheet can significantly affect the movement of a wave packet, and for $T > T_f$ it does not significantly affect the movement of wave packet. We analyzed the functional dependence of the temperature T_f on the shape and the size of the sheet. It is very interesting under which conditions the temperature T_f is high enough to store hydrogen. Approximate quantum Newton's equation was used for calculating

$$\frac{d^2\eta}{dt^2} = -\frac{\partial U}{\partial \eta} - \frac{1}{8}\frac{\partial^3 U}{\partial \eta^3}\delta^2, \qquad (1)$$

where η= x,y,z are the radius vector components of the molecule wave packet centre, U is potential energy of interaction approximated by the Lennard-Jones potential, and δ is the width of the molecule wave packet assumed to be constant for the particular experiment. Placing δ=0 in approximate quantum Newton equation, this equation reduces to ordinary Newton equation of motion. Varying the number of carbon atoms comprising the sheets: N_C = (2+2N)·(4+4N), and shape which is described with angle β, we observed the trajectories of the wave packet. In this way β gives us the radius of curvature R

$$R = \frac{(3N+2)a}{\beta} \qquad (2)$$

where a = 0,142 nm.

3. TEMPERATURE DEPENDENCE ON THE GRAPHENE SHEET SHAPE

From the graphics presented in Fig.3, it can be seen that for different shapes of the graphene sheet there is a different temperature interval favourable for hydrogen storage. For graphics a) and b) there is good agreement with GBE, for $\beta = 0...0{,}5\pi$ that is temperature interval between 100K and 600K and for $\beta = 0...0{,}25\pi$ that interval is between 250 K and 450 K. For graphic c) there is no agreement with GBE.

4. CRITICAL TEMPERATURE DEPENDENCE ON GRAPHENE SHEET SIZE

From the graphics presented in Fig.4 it is evident that for different sizes of the graphene sheet there are different temperature intervals favourable for hydrogen storage. The results obtained in our experiments show good agreement with GBE. Also it should be mentioned that a small change of initial conditions results in a noticeable change of temperature interval. From the figures presented above we can conclude that for $N = 6..15$ number of carbon atoms there is favourable temperature interval between 100K and 500K, something that is very useful in industry.

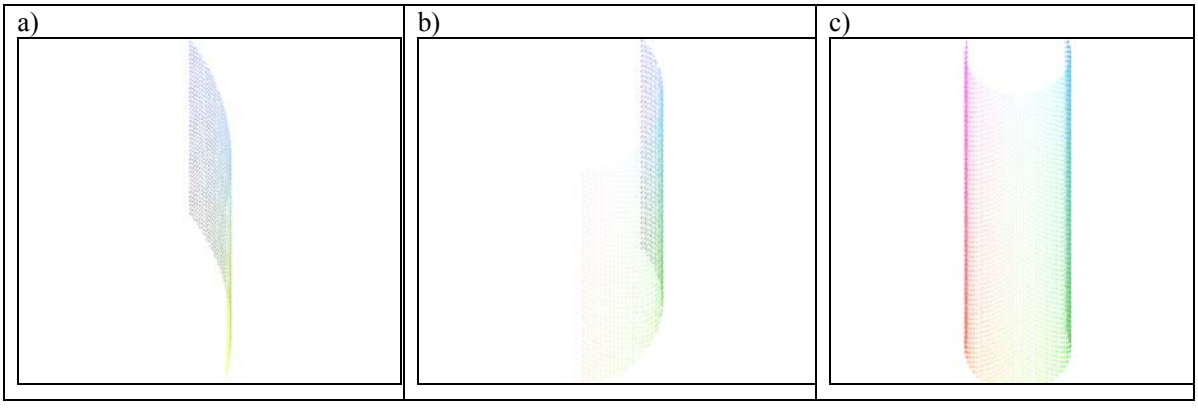

Figure 1. Appearance of graphene sheet for :
a) $N = 20$, $\beta = 0{,}3\pi$, b) $N = 20$, $\beta = 0{,}7\pi$, c) $N = 30$, $\beta = 1{,}2\pi$,

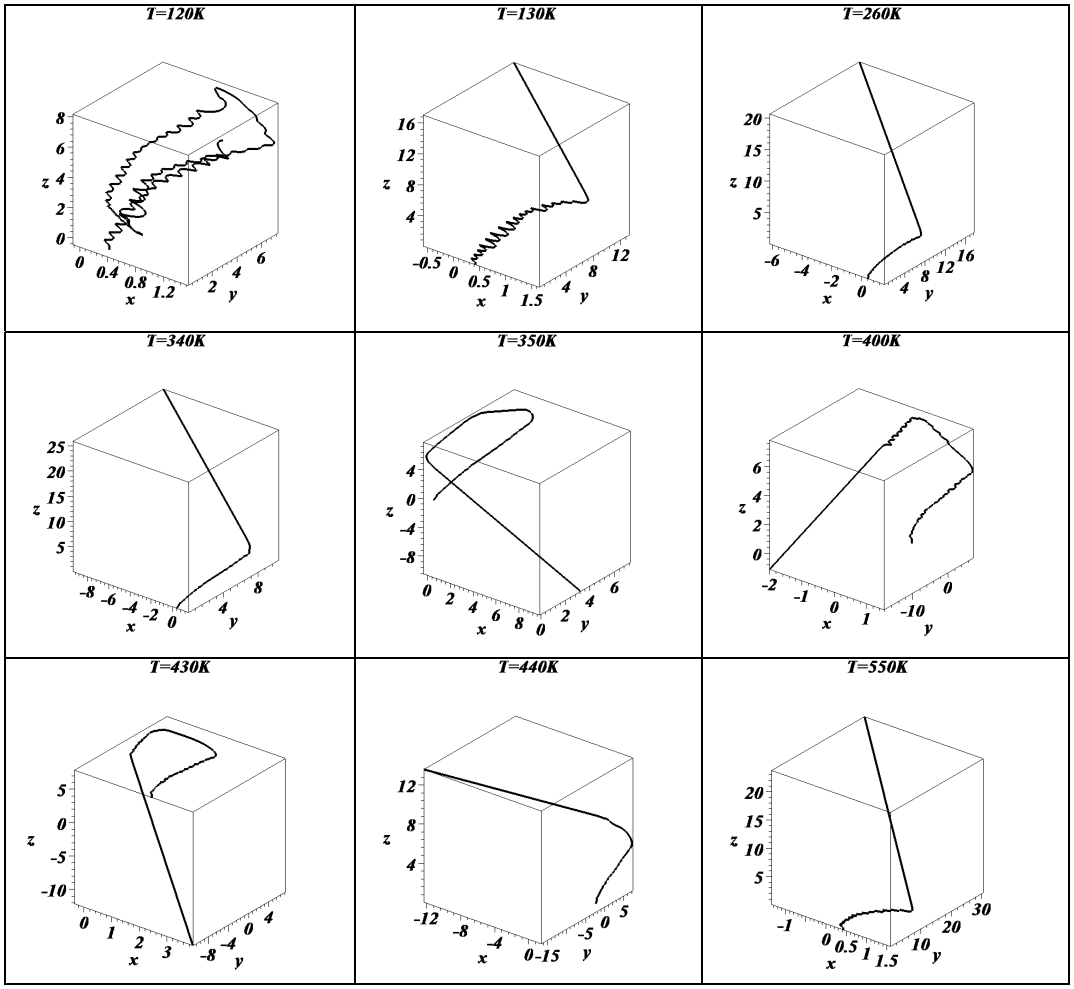

Figure 2. Trajectories of the wave package center for $N=15$, $\beta=0{,}1\pi$, $\delta=0{,}005$, $x(0)=2{,}95\,a$, $y(0)=0{,}2\,a$, $z(0)=0{,}15a$, $V_x(0)=0$, $V_y(0)=V_z(0)=\sqrt{\dfrac{4kT}{\pi m}}$. *Here* $T_{\mathrm{f}}=430K$.

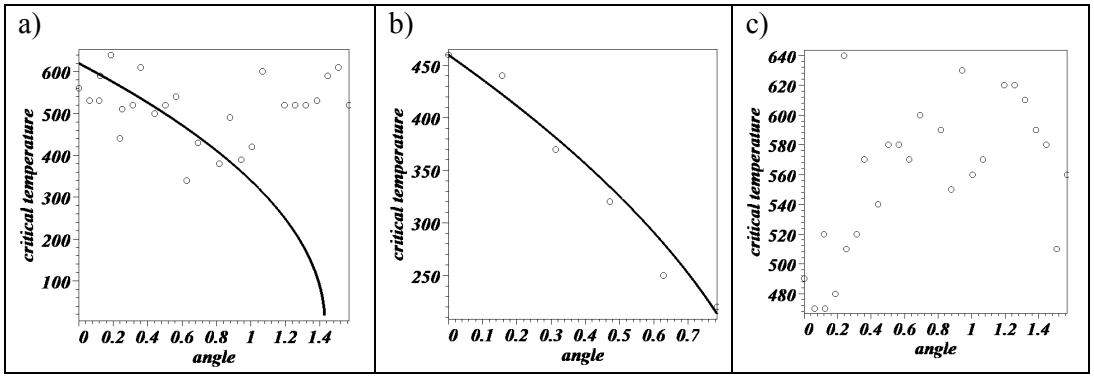

Figure 3. Temperature dependence of the graphene sheet shape for:

a) $N=11$, $\beta=0\cdots0{,}5\,\pi$, $f(\beta)=660\cdot\sqrt{1-\dfrac{2{,}5\,\beta}{N}}$, $y(0)=0$, $\delta=0{,}005$;

b) $N=10$, $\beta=0\cdots0{,}25\,\pi$, $f(\beta)=460\cdot\sqrt{1-\dfrac{10\beta}{N}}$, $y(0)=0$, $\delta=0{,}005$;

c) $N=11$, $\beta=0\cdots0{,}5\,\pi$, $y(0)=0{,}3\,a$, $\delta=0{,}005$.

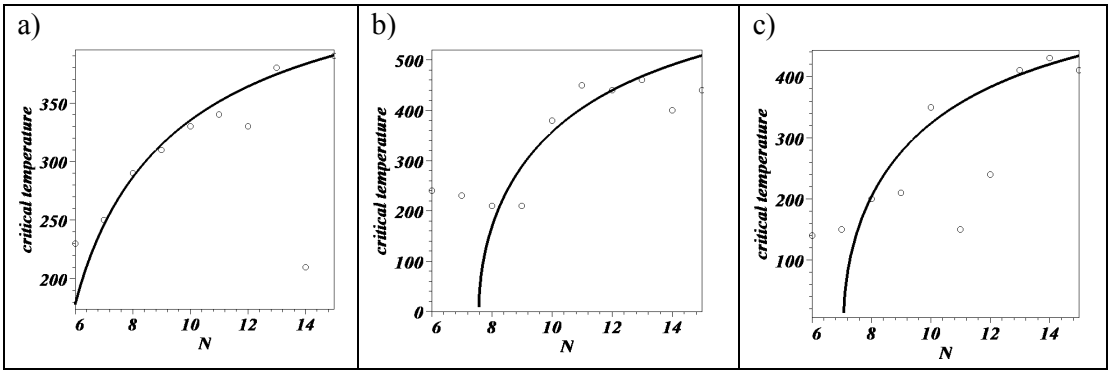

Figure 4. Temperature dependence of the graphene sheet size for:

a) $N = 6,7,...15$, $\beta = 0,15\,\pi$, $\delta = 0,005$, $y(0) = 0$, $f = 483 \cdot \sqrt{1 - \frac{11\beta}{N}}$;

b) $N = 6,7,...15$, $\beta = 0,05\,\pi$, $\delta = 0.005$, $y(0) = 0$, $f = 690 \cdot \sqrt{1,1 - \frac{53\beta}{N}}$;

c) $N = 6,7,...15$, $\beta = 0,15\,\pi$, $\delta = 0,005$, $y(0) = 0,15\,a$, $z(0) = 0,05\,a$, $f = 597 \cdot \sqrt{1 - \frac{15\beta}{N}}$.

5. AL – ADSORBED GRAPHENE

Surya et al. have studied the behavior of graphene and C_{60} with adding of the additives. They have shown that the large radius single walled carbon nanotube (SWCNT) functionalized with boron can have appreciable hydrogen storage capacity [5]. Here we consider motion of a hydrogen molecule near a graphene layer with $(N+1)^2$ Al atoms adsorbed on both sides. The initial conditions are: $x(0) = 3\,a$, $y(0) = 0,1\,a$, $z(0) = 0,7\,a$, $V_x(0) = 0$, $V_y(0) = V_z(0) = \sqrt{\frac{4kT}{\pi m}}$. The obtained results are presented in Table 1.

We see that Al-adsorbed graphene is more appropriate for hydrogen storage than clean graphene, in agreement with [6].

Table 1. Comparison of the critical temperature values (K) for clean graphene and Al-adsorbed graphene.

N	$\beta(\pi)$	T_f (without Al)	T_f (with Al)
6	0	220	250
7	0,1	230	280
8	0,15	450	450
9	0,3	300	350
9	0,55	400	440
11	0,55	540	550
11	0,09	200	290

6. CONCLUSION

Investigating the most favorable conditions for the storage of hydrogen are the main preoccupations of today's scientific research. A good understanding of the interplay between molecular physical adsorption and atomic chemical adsorption would be useful in terms of addressing the problem of hydrogen storage, as well as for understanding the fundamental issues, such as the puzzle of how H_2 is formed in the interstellar medium. In particular, graphite is an attractive candidate for hydrogen storage due to its properties of being cheap, chemically inert and environmentally-friendly. In this paper we have observed the interactions of graphene sheet with one wave packet. We should mention that our computational experiments have some shortcomings, the principle ones being: (1) a relatively small number of C atoms are considered; (2) C atoms are always placed in their equilibrium positions; (3) changes of the wave packet width are neglected; (4) only one hydrogen molecule and one graphene sheet interaction is considered.

Functional dependence of the temperature T_f on the shapes and sizes of sheet has been analyzed. It is very interesting under which conditions the temperature T_f is sufficiently close to room temperature and favorable for hydrogen storage. Also, the presence of impurities adsorbed on graphene surface and their influence on studied temperature change are very important. From our experiments we have concluded that for certain small curvature of graphe-

ne sheet ($\beta = 0...0{,}5\pi$) we can obtain a relatively favorable temperature range for storage of hydrogen. Something that is very important is that this temperature range was relatively easily achieved under normal conditions. For a relatively small number of C atoms in our case, 10 and 11, the interval is between 400 and 650 K. Especially favorable conditions for storing hydrogen can be obtained by adding small amounts of graphene impurity. In our case it was aluminum. From the obtained results we can conclude which is the favorable interval around the room temperature, and we know that most of the present-day scientific efforts focus on obtaining the optimal storage conditions.

7. REFERENCES

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МЕЂУДЈЕЛОВАЊЕ ТАЛАСНОГ ПАКЕТА И ГРАФЕНСКОГ ЛИСТА И КРИТИЧНА ТЕМПЕРАТУРА СКЛАДИШТЕЊА ВОДОНИКА

Сажетак Испитивање карактеристика наноматеријала веома је важно за примјену у индустрији. Изучавање особина графена је важно за складиштење водоника. У раду је проучавано међудјеловање таласног пакета који описује молекул водоника и графенског листа. Одређивана је температура T_f, гдје за $T \leq T_f$ графенски лист може знатно да утиче на кретање таласног пакета, а за $T > T_f$ битно не утиче на кретање таласног пакета. Посматрана је функционалана зависност температуре T_f од облика и величине листа. Веома је интересантно под којим условима је температура T_f погодна, тј. довољно близу собне температуре за практично складиштење водоника. Рјешавана је апроксимативна Њутнова квантна једначина. Резултати добијени рачунарским експериментима помоћу Рунге–Кута–Фелбергове методе, дјелимично се слажу са једначином коју су предложили Гизбир и Бишело. Они су разматрали зависност величине и облика наноструктуре (графенског листа) и карактеристичних температура (фазних) прелаза, предлажући универзалну једначину, гдје се наши резултати могу фитовати кривом таквог облика за одређене температурне интервале.

Кључне ријечи: графен, складиштење водоника, Њутнова квантна једначина.

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