INFLUENCE OF MIGRATION THE RADIATION-INDUCED EXCITATIONS IN HETERO-FULLERENES $C_{58}Si_2$ AND $C_{68}Si_2$ OF THEIR PROBABILITY OF DAMAGE

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ABSTRACT

Theoretically investigated the role of migration of radiation-induced excitation in the damaged hetero-fullerenes C58Si2 and C68Si2. Defined expressions for the probability collapse of fullerenes different structures. Investigate the changing probability on irradiated conditions.

Key words: irradiation, energy migration, probability of collapse, hetero-fullerenes.

INTRODUCTION

Physical properties of materials under irradiation significantly changed, due to changes in the microstructure of this material. One result of the impact of exposure to the material is radiation-induced excitation of the electron subsystem of molecules matter [1-4].

In a molecule such transfer occurs repeatedly, and energy can shift from place of absorb on relatively large distance [5]. On moving, excitation energy dissipated in each between the atomic transition.

In the presence in a molecule atoms of several varieties can be expected that the energy bind of different sorts of atoms will be different, while some will be more strongly linked that other less. In some cases the difference of energy strong coupling and weak will be significant. We can expect that the vagus excitation, which arose due on the strong bind, reaching the weak, break it, resulting in damage or collapse of the molecule.

Thus, of interest to investigate the lifetime and the likelihood of damage to the molecules, in which are formed vagus excitation, and to identify the basic patterns are caused by this process.

Thus, if there is a walk of excitation, the probability of damage (collapse) of the molecule depends on the mechanisms of migration of energy to a large extent depends on its structure, the number of weak binds, and the configuration of the placement of weak binds in the molecule. Another important factor that affects the probability of collapse of the molecule is the

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energy of initial excitation, which determines the maximum length path of migration of excitation to the moment of its complete decay.

In this work the probability of damage of the Herero-fullerenes $C_{58}Si_2$ and $C_{68}Si_2$ [6-7] depending on the structure of molecules, initial excitation energy, the number and configuration of weak binds.

RESULTS AND DISCUSSION

Results of numerical calculations of the probability of collapse of the herero-fullerenes $C_{58}Si_2$ and $C_{68}Si_2$, depending on the excitation path, and placement configurations of impurity atoms are represented in the graphs in *Fig. 1-2*, respectively. The calculations were carried out at values of energy bonds: Si-C - 290 kJ/mol, C-C - 344 kJ/mol and independent placement of atoms Si. Length of run, on condition of exponential decay of the excitation path length was defined expressions:

$$n = \frac{x_0}{h} \ln\left(\frac{E_0}{E_{\min}}\right),$$

where, n is number of excitation jumps, x_0 is distance at which the excitation energy decreases in e times, h is distance between neighboring atoms, E_0 is initial value of excitation energy, $E_{\min}$ – minimum energy at which the gap weak connection is still possible.

Magnitude L – distance between atoms Si (in units of interatomic distance). Ortho and meta configuration [7] correspond to the case when Si atoms are in the neighborhood.

Based on the results can be noted that with increasing length of run initial perturbation probability of damage of hetero-fullerene as $C_{58}Si_2$ and $C_{68}Si_2$ increases, approaching to the one.

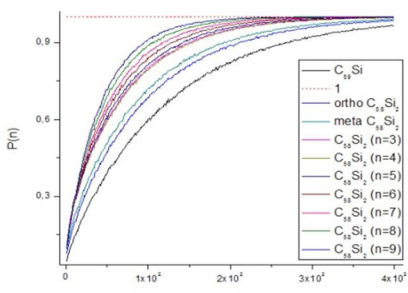

Fig. 1 – The probability of damage hetero-fullerene C58Si2 depending on the initial excitation energy and configuration placement of weak ties

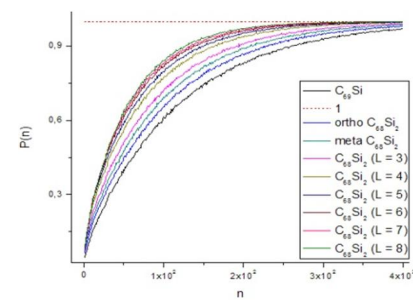

Fig. 2 – The probability of damage hetero-fullerene depending on the initial excitation energy and configuration placement of weak ties

Change of configuration the placement of weak ties also lead to a change in the probability of collapse of the molecules. In particular, with increasing distance (L) between the atoms replacing possibility damage Herero-fullerenes also increases.

CONCLUSIONS

Based on the assumption that the radiation excitation of electron subsystem of atoms can wander through the molecule and outrage break weak binding, using numerical methods, built graphics of damage herero-fullerenes $C_{58}Si_2$ and $C_{68}Si_2$ depending on the energy of the initial disturbance.

Investigated the influence of configuration placing weak bonds on the probability of damage of hetero-fullerenes$C_{58}Si_2$ and $C_{68}Si_2$.

Determine the average time of impact to radiation, after it is off.

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