INTRODUCTION

One of the main goals in nanophysics and nanotechnologies is the synthesis of fundamentally new substances with required properties from the known elements of the Periodic Table. The “building block” of such a substance is a cluster consisting of a small number of atoms (and having a size on the order of a nanometer) and having the structure and properties radically differing from those of the conventional condensed substance.

If clusters are combined into an ensemble so that they preserve their individual properties while remaining bound to one another, they form a new material (nanosubstance). A brilliant example is the carbon cluster fullerene C_{60} discovered in 1985 [1]. An ensemble of fullerenes (fullerite) possesses a large number of unique properties. For example, fullerenes exhibit ferromagnetism [2] and superconductivity [3], while familiar carbon structures such as graphite and diamond are semiconductors.

The question arises: is it possible to synthesize a nanosubstance capable of storing and releasing large amounts of energy? Large demand existing at present in the new type of energy carriers is due to a considerable gap between the characteristic energies of chemical and nuclear energy carriers. Another question: which chemical elements should be used to obtain HEDM? In this study, we give the following answer to these questions: it is possible in principle to synthesize clusters of helium, viz., an element that does not form a condensed substance under normal conditions (i.e., at room temperature and under atmospheric pressure).

We predict the existence of a metastable cluster consisting of four helium atoms and prove that the energy accumulated in the cluster exceeds the energy of available chemical energy carriers by more than an order of magnitude (preliminary results were published in [4]). The structure and energy parameters of the cluster and its stability and lifetime are studied in detail from first principles. It is shown that the energy accumulated in the cluster is released virtually completely during decomposition into individual helium atoms. This means that helium clusters are a promising material with a high accumulated energy density (HEDM). © 2005 Pleiades Publishing, Inc.
according to terminology proposed in [4]). The energy stored in type II clusters is released during decomposition of clusters into molecules or individual atoms. Note that most chemical elements form type I clusters (see [4]) whose binding energy increases with the number of atoms in a cluster, while the accumulated energy is released upon merging of small clusters into large ones.

It was noted earlier in [4] that type II clusters are formally analogous to heavy metastable nuclei (e.g., uranium), while type I clusters are analogous to light nuclei (e.g., deuterium). Indeed, the binding energy of heavy nuclei decreases upon an increase in the number $N$ of nucleons in the nuclei, while the energy is released during nuclear fission. On the contrary, the binding energy in light nuclei increases with $N$, making nuclear fusion advantageous from the energy point of view. We studied the properties of type I and II clusters theoretically in [4] using carbon and nitrogen clusters, respectively, as examples.

As motivation for such a choice of chemical elements, let us consider the total energy $E(\{R_i\})$ of a cluster consisting of $N$ atoms as a function of coordinates of all atoms, $\{R_i\}$, $i = 1, \ldots, N$. The minima of $E(\{R_i\})$ correspond to different structures that can be formed by these atoms. The global minimum with the lowest energy $E_0$ corresponds to the so-called ground state of the system. This minimum is restricted by an infinitely long barrier ensuring an infinitely long lifetime in the ground state. It should be noted that the lifetime $\tau$ of a metastable structure is finite since there is a finite probability of transition of the system to the ground state with release of energy $E_{\text{acc}} = E_p - E_0$ stored in the metastable state. It should be noted that the lifetime $\tau$ of a metastable structure may be very long (e.g., many years in the case of diamond) since the quantity $\tau$ is an exponential function of temperature, $\tau(T) = \tau_0 \exp(U/k_BT)$, where $U$ is the height of the energy barrier separating the metastable state from the ground state, $\tau_0$ is a microscopic value on the order of 1 fs–1 ps, and $k_B$ is the Boltzmann constant.

Since nitrogen, oxygen, and hydrogen, as well as noble gases (like helium), do not form a condensed substance under normal conditions (we disregard condensation due to very week Van der Waals forces), we can assume that clusters of these elements do not possess a global minimum of the total energy $E(\{R_i\})$. At the same time, local minima (if they exist) must obviously be formed for relatively high energies (otherwise they would have been observed experimentally). It follows hence that, first, metastable structures of helium, nitrogen, and other elements of this group must accumulate large amounts of energy and, second, release of energy during a transition from a metastable to the ground state must take place during decomposition of clusters into atoms (e.g., He) or molecules (e.g., $N_2$). This leads to virtually complete release of accumulated energy, which is a considerable advantage of such structures as prospective energy carriers.

The available experimental and theoretical data indicate that helium atoms in the ground state do not form clusters $\text{He}_n$ ($n = 2, 3, 4, \ldots$) with covalent bonds. However, it was demonstrated experimentally in [5] that a metastable covalently bound cluster (triplet molecule) $\text{He}_2^*$ in the excited state $3\Sigma_u^+$, which was studied theoretically in [6, 7], exists. Figure 1 shows schematically the filling of orbitals of the $\text{He}_2^*$ molecule with electrons. Three electrons occupy “inner” orbitals formed by atomic 1s orbitals, while the fourth electron is on the “outer” excited orbital formed by atomic 2s orbitals. It is important to note that the $\text{He}_2^*$ molecule is in the triplet state with total spin $S = 1$ (see Fig. 1), which increases its stability and lifetime due to the prohibition on recombination imposed by the Pauli exclusion principle.

The triplet $\text{He}_2^*$ molecule accumulates energy approximately equal to 9 eV/atom and releases this energy during decomposition into helium atoms. This was confirmed experimentally in [5]. Thus, the $\text{He}_2^*$ molecule may play the role of a building block whose properties radically differ from the properties of conventional helium. The question arises: can an ensemble