

Development of nanosensors in nuclear technology

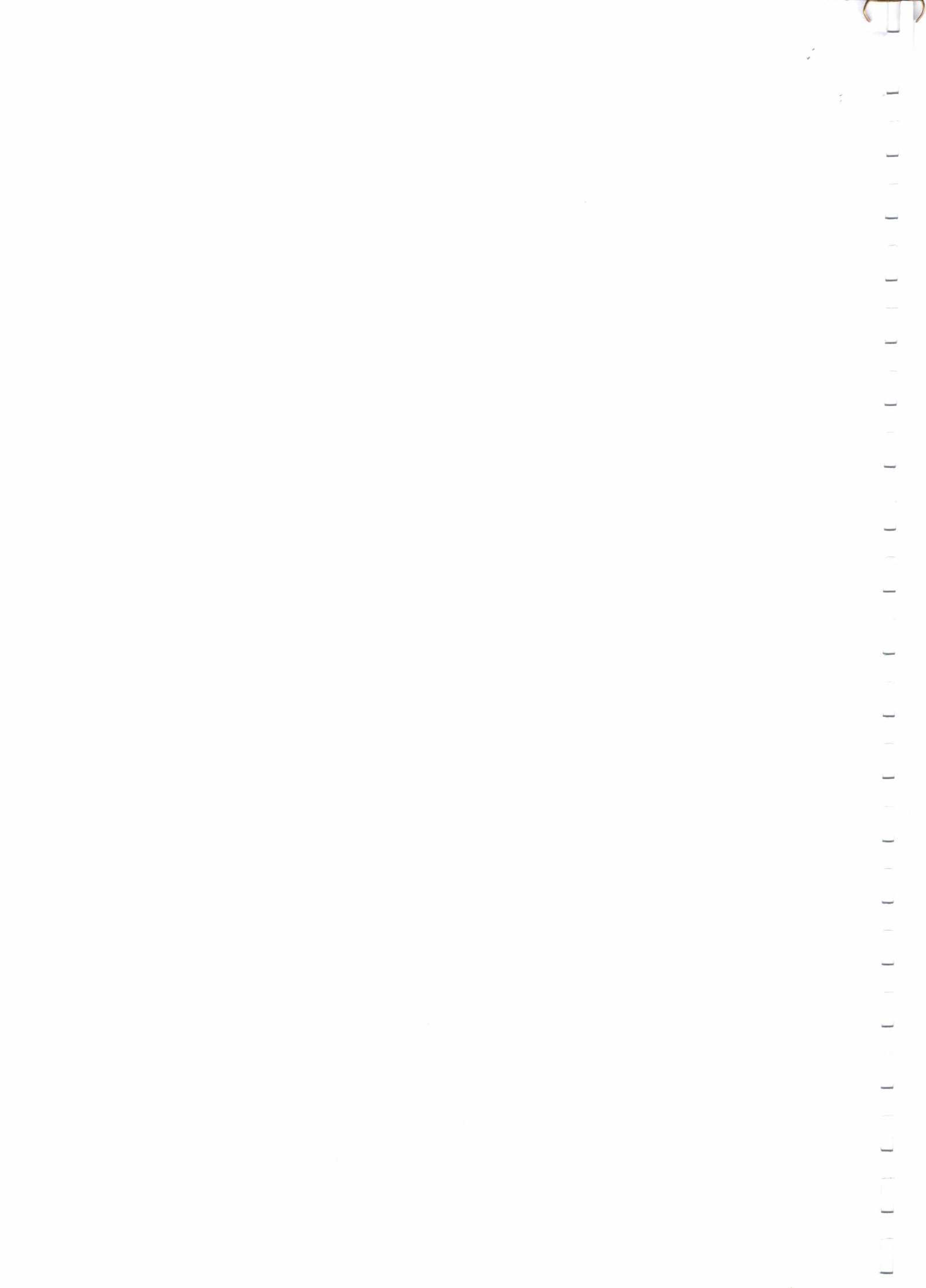
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Development of Nanosensors in Nuclear Technology

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Abstract. Selectivity, sensitivity, and stability (three S parameters) are developed as a new range of sensor this provided instruments for harsh, radioactive waste polluted environment monitoring. Isotope effect is very effective for nuclear radiation sensors preparation. In this presentation are reviewed of the development of Nanosensors in nuclear technology, such as high temperature boron and its compounds with suitable physical and chemical features as sensitive element for temperature and nuclear sensor, Boron isotopes based semiconductor nanosensors and studies of the mechanism of the removal uranium from radioactive wastewater with graphene oxide (GO).

INTRODUCTION

As the theme of this presentation, the words by Richard Feynman: "I will not now discuss how we are going to do it, but only what is possible in principle – in other words, what is possible according to the laws of physics" [1]. Just after Christmas 1959, he delivered a now-famous talk – titled "There's Plenty of Room at the Bottom" – at the California Institute of Technology. It is possible, he proposed, for scientists to assemble new materials at the level of single atoms and molecules, where there are "new kinds of forces and new kinds of possibilities, new kinds of effects". It is generally accepted that Feynman's visionary discussion of the problems and promise of miniaturization constituted the starting point for the new field that today is called *Nanotechnology*.

Nanobiosensors, optical nanosensors and magnetic nanosensors, with many technical details are reviewed by many researchers. Here, we present an overview of all nanosensors, showing similarities and fundamental differences among the various categories. The aim of this review is to provide an overview, which is suitable for beginners to realize the growing importance of this field. Nanosensors are sensing devices with at least one of their sensing dimensions being less than 100 nm. In the field of Nanotechnology, nanosensors are instrumental for (a) monitoring physical and chemical phenomena in regions difficult to reach, (b) detecting biochemicals in cellular organelles and (c) measuring nanoscopic particles in the industry and environment. A search on the terms "nanosensor(s)" and "nano-sensor(s)" appearing in titles of journal papers shows a growing trend in nanosensor research, as evident from the resulting publication record. Needless to say, a far greater number can be expected if a complete keyword search is performed to include all nanosensor publications. The advance in scientific understanding is naturally followed by technological development. Although sensors have a long and illustrious history, the realm of nanosensors is relatively new.

Table 1 refers to the development of various nanosensors. Figure 1 refers to the various nanosensors can be loosely grouped into three broad categories of nanosensors:

- Optical nanosensors
- Electromagnetic nanosensors
- Mechanical and/or vibrational nanosensors.

TABLE 1. The development of nanosensors.

Years	Nanosensors	Reference	Years	Nanosensors	Reference
1994	Mechanical	2	2004	Nanogap nano-particle	18
				Magnetic nano-particle	19
1996	Optical	3	2005	FRET based	20
				Magnetic based	21
				Semiconductor and piezoelectric	22
				Localized surface plasma	23
				resonance nanosensor	24
1998	Optical Fiber Liposomal	4	2007	PANI-CNTs	26
		5		calorimetric biosensors	27
1999	Polymer beads Nanoelectrode	6	2010	PANI-MWNTs gas sensors	28
		7			
2001	Nanowire Magnetic	8,9	2011	PANI-SWNTs chemosensory Amperometric biosensors	29
		10			30
2002	PEBBLE Quantum dot Ion channel Nanoribbon	11	2013	Piezo-electric biosensors	31
		12			
		13			
		14			
2003	C-60 Nanocrystal Super conducting	15	PEBBLE(photonic Explorers for Bioanalysis with FRET (Fluorescence Resonance Energy Transfer) Biologically Localized Embedding)		
		16	MWNTs(Multiple Wall Nanotubes)		
		17	SWNTs(Single Wall Nanotubes)		

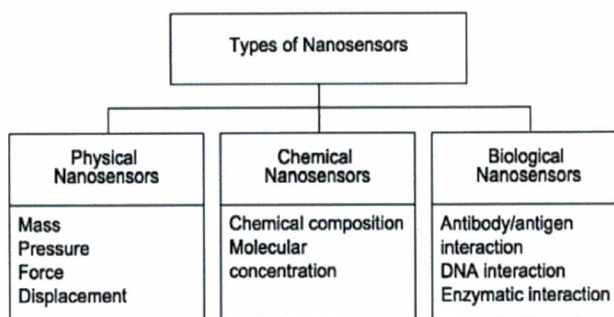


FIGURE 1. Types of nanosensors.

NANOSENSORS DEVICES

Graphene and its derivatives are one of novel nanomaterials, namely, Graphene Nanoribbons (GNRs) and Carbon Nanotubes (CNTs) [32] and graphene oxide [33] provide outstanding sensing capabilities and are the basis for many types of sensors [34]. Based on the nature of the measured magnitude, nanosensors can be classified as follows:

Physical Nanosensors

Mass, pressure, force, or displacement is usually based on the fact that the electronic properties of both nanotubes and nanoribbons change when these are bent or deformed [35]. For example, a CNT can be used to build a field-effect transistor (FET) nano in size, the Nano tube dimensions are main effective for on/off threshold on, shape and temperature amongst others. A local deformation of the tube creates a change in the on/off threshold voltage of the transistor. Starting from this simple principle, different types of Nano-Electromechanical Systems (NEMSs) have been proposed in the literature with different applications, such as pressure nanosensors [36], force nanosensors [37] or displacement nanosensors [38].

Chemical Nanosensors

These are used to measure magnitudes such as the concentration of a given gas, the presence of a specific type of molecules, or the molecular composition of a substance. The functioning of the most common type of chemical nanosensors is based on the fact that the electronic properties of CNTs and GNRs change when different types of molecules are adsorbed on top of them, which locally increase or decrease the number of electrons able to move through the carbon, lattice [39]. Similarly to physical sensors, when a nanotube or a nanoribbon is used in a transistor configuration, the presence of a specific type of molecules changes the on/off threshold voltage of the transistor [40][41]. For the time being, hundreds of chemical nanosensors based on this simple principle have been manufactured with different specific detection targets [39].

Biological Nanosensors

These are used to monitor biomolecular processes such as antibody/antigen interactions, DNA interactions, enzymatic interactions or cellular communication processes, amongst others. A biological nanosensor is usually composed of (i) a biological recognition system or bioreceptor, such as an antibody, an enzyme, a protein or a DNA strain, and (ii) a transduction mechanism, e.g., an electrochemical detector, an optical transducer, or an amperometric, voltaic or magnetic detector [42]. There are mainly two subtypes of biological nanosensors based on their working principle: electrochemical biological nanosensors and photometric biological nanosensors. The elec-trochemical biological sensors work in a similar way to chemical nanosensors, but in this case, the change in the electronic properties of, for example, a CNT-based FET transistor, is induced either by:

- A protein or any other chemical composite that binds itself to the functionalized nanotube [43].
- A specific antigen that binds itself to an antibody glued to the nanotube [44].
- A single stranded DNA chain that binds itself to another DNA chain which has been attached to the nanotube [14].

Nanosensors able to detect lung cancer, asthma attacks, different common virus such as the influenza virus, or the parasite responsible for malaria which have been already successfully manufactured [45][46]. The second subtype of biological nanosensors is based on the use of noble metal nanoparticles and the excitation using optical waves of surface plasmons, i.e., coherent electron waves at the interfaces between these particles. Simply stated, the resonant frequency of the surface plasmons resulting from light irradiation changes when different materials are adsorbed on and in between the particles. This technique, known as localized surface plasmon resonance (LSPR), is the underlying principle behind many biological nanosensors [47][48]. One of the main constraints of this sensing mechanism is the requirement of an external source of light and a device which is able to measure and compare different resonant frequencies of the particles. We believe that this can be overcome by means of coordination and communication among nanosensors. For example, nanosensors could locally irradiate the same particles with a much lower power and measure the reradiated energy at different frequencies. The result of this operation could then be processed or forwarded to a data sink.

In Figure 2, the basic working principle of the three main types of nanosensors are shown. In Fig. 2(a), an unperturbed field-effect transistor based on a carbon nanotube is given. A CNT-based FET is mainly composed of a nanotube suspended over two electrodes.

Assuming that the CNT has the adequate geometry to behave as a Semiconducting material ¹⁶, electrons from the source will be able to reach the drain only if energy above the conducting threshold is applied on the nanotube. This threshold can be altered either when the tube is bent, Fig. 2(b); when the amount of free charges on the tube is increased or decreased by the presence of donor or acceptor molecules of specific gases or composites, Fig.2(c); or when the tube has been functionalized with a biological receptor such as an antibody and this is bound to the specific antigen of a given disease, locally changing the number of electric charge in the tube, Fig. 2(d).

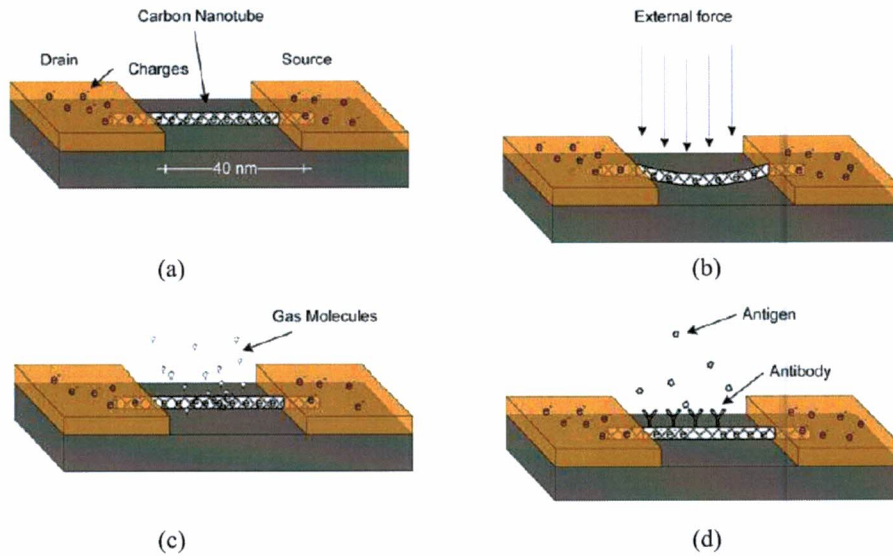


FIGURE 2. CNT-based physical, chemical and biological nanosensors [49]: (a) CNT-based FET transistor, (b) Physical nanosensor, (c) Chemical nanosensor, (d) Biological nanosensor.

BASIC CHARACTERISTICS OF CHEMIRESTOR GAS SENSORS

The electrical resistance of a chemiresistive sensor change drastically (increase or decrease) when exposed to the molecules of analyzing gas. Increase or decrease in resistance depends on the nature of sensor material (n-type or p-type) and the gas (reducing or oxidizing). Atypical response curve, that is, variation of resistance of sensor with time of exposure and with drawal of analyzing gas is schematically depicted in Figure 3.

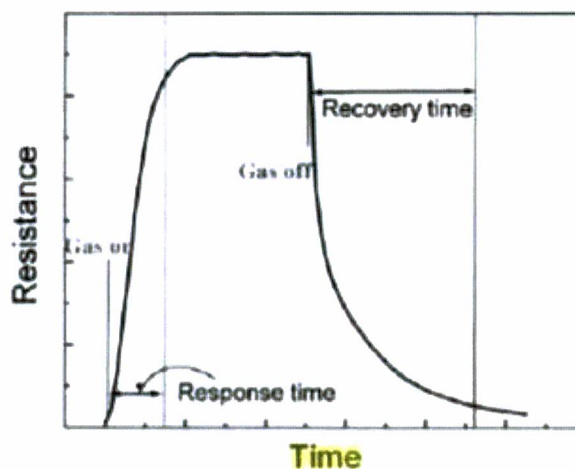


FIGURE 3. Response curve of a chemiresistive gas sensor.

The response curve of sensor is characterized by following five parameter (Sensitivity, Response time, Recovery time, Selectivity and Longtime stability) [50].

Sensitivity

The Sensitivity (S) of a sensor can be defined by many ways. The often used definitions of S are the following:

- A ratio of resistance in air $R(\text{air})$ to that in gas $R(\text{gas})$

$$S = \frac{R(\text{air})}{R(\text{gas})} \quad (1)$$

A high value of S for a particular gas indicates that the material is very good sensor.

- Sensitivity percentage

$$S(\%) = \frac{R(\text{air}) - R(\text{gas})}{R(\text{gas})} \times 100 \quad (2)$$

A positive value of S implies film resistance decrease on gas exposure and vice versa.

Response Time

The response time is the time interval over which resistance attains fixed percentage (usually 90%) of final value when the sensor is exposed to full-scale concentration of the gas⁵⁰.

Recovery Time

This is the time interval, usually referred as T_{10} , over sensor resistance reduces to 10 % of the saturation value when the sensor is exposed to full-scale concentration of gas and then placed in the clean air. A good sensor should have a small recovery time so that sensor can be used over and over again.

Selectivity

Usually most chemiresistive sensors exhibit significantly high value if sensitivity for many gases under similar operating conditions. The selectivity or specificity of sensor towards an analyzing gas is expressed in terms of dimension that compares the concentration of the corresponding interfering gas that produces the same sensor signal. This factor is obtained by:

$$S = \frac{\text{Sensitivity of the sensor for interfering gas}}{\text{Sensitivity toward the desired gas}} \quad (3)$$

Long term stability

This is the ability of the sensor to maintain its properties when operated continuously for long duration in hostile environment. The good sensors are expected to work for several years without showing a drift in any of the above four parameters. All these five parameters depend on the sensing material, the interaction between the gas and sensor, the sensor operating condition etc. In order to control these parameters, scientific understanding of gas-sensor interaction, and various new technological concepts and novel materials have been developed.

BORON ISOTOPES BASED SEMICONDUCTOR NANOSENSORS

Radioactive pollutants generated directly or indirectly, as a result of nuclear waste influence on different substances working in nuclear power stations (water, gases, metals, etc.) or existing nearby radioactive materials places. The need is for devices that can achieve the necessary sensitivity at a cost that will not prohibit their widespread deployment and with the capabilities to provide quantitative information as well as alarm functions.

These devices and particularly detectors of nuclear radiation with autonomous energy supply are very useful for illumination and prevention of nuclear materials illegal transportation and transfer. The development of new range of sensors has provided instruments with enhanced selectivity and sensitivity for harsh, radioactive waste polluted environment monitoring [51].

By two major competitive research groups making gamma and neutron radiation detectors (sensors): first was Lawrence Berkeley National Laboratory Semiconductor Detector Group and second is the USSR's Middle Machinery Ministry (comprising Kurchatov Institute of Atomic Energy, Giredmet Institute of Rare Metals, Institute of Radioisotope Devices, etc.), where focused on the development of semiconductor-based radiation detectors and their applications. The best sensor material for gamma radiation sensors was, and still is, ultrapure Ge and Si or Ge doped by Ga impurities with acceptor concentration up to 10^{16} cm^{-3} . For neutron radiation measurement the B isotopes contained Si was developed [52]. Isotope effect is very effective for nuclear radiation sensors preparation.

Today, nuclear radiation detection systems exist utilizing a variety of solid state detectors. The solid state detectors are based on semiconductor material such as silicon, germanium, cadmium telluride, zinc oxide, etc. A major advantage of such detection systems is their extremely high energy resolution. Another prospective application of isotope effects is their utilization in quantum spin based devices. In the last years the strong attention was paid to development of so called "high temperature boron and its compounds because of their suitable physical and chemical features as the sensitive elements for temperature and nuclear radiation sensors. They are semiconductor materials (mainly boron and boron carbide) with a high melting point, mechanical/ chemical strength in corrosive media and strong atomic bonds providing high stability in the radiation area.

To raise its radiation resistance under neutron irradiation, boron should be enriched with ^{11}B isotope. In case of semiconductor Boron based elements preparation enriched by ^{10}B following n, α nuclear reaction it is possible to build a very sensitive neutron detectors [53].

Last decades P. J. Kervalishvili research group [54] started the work to develop novel boron-based nanosensory elements for temperature and neutron sensors that can operate in harsh environments (corrosive media, nuclear radiation, etc.) Boron is a wide-range high temperature semiconductor with a prohibited energy zone of about 1.6 eV. Boron carbide (B₄C) and some other boron rich compounds have a similar forbidden energy gap, which defines their electrical resistance. High mechanical and chemical strength in various corrosive media, and the possibility to change the isotope content from ^{11}B to ^{10}B in almost every concentration range, allows to improve the radiation resistance of boron based sensors and nanosystems.

Boron (and its compounds) crystalline and compact pellets are possible to be prepared by different metallurgical methods: vacuum synthesis, melting zone, free crystallization, vacuum hot pressing, sintering hot compaction, self-propagation high-temperature synthesis, gasostatic pressing, etc. Study of their properties such as the temperature resistance, voltage-current characteristics, ice melting point sensitive response, structural stability, etc. showed a high temperature resistance coefficient and linearity of voltage-current parameters within their operational range. Using such approaches researchers have managed to produce compact pellets made of boron, boron carbide and aluminum dodecaboride etc. Typically, the pellets had a cylindrical or thick disk shape, high density, low concentration of metallic impurities, and room temperature electrical resistance in the range $10^6 - 10^8$ Ohm.m. One more advantage of boron and its compounds is the preparation of sensitive elements in types of ceramic thin films, nanostructured elements, quantum dots and other nanosystems, which make possible to obtain different properties materials and sensitive elements [55][56][57].

Temperature dependence of boron, boron carbide and aluminum dodecaboride electric resistance was studied in 150-750 K temperature range. A thermostat provided the temperature constancy by the following transient phases: melting, boiling and eutectics solidification. The points corresponding to the eutectic solidification temperatures were obtained using aqueous solutions of the eutectic composition, which form cryohydrates coinciding with the liquid phase by their composition. A Chromel-Alumel thermocouple and a platinum resistance-thermometer measured the temperature at the constant point. The electric parameters of the sensitive elements were measured with a measuring

bridge circuit. The example of temperature dependence of the resistance of the aluminum dodecaboride enriched by ^{11}B is shown at the Figure 4.

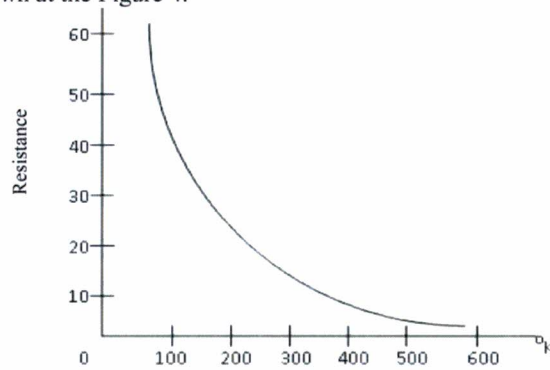


FIGURE 4. Temperature dependence of the electroresistance of AIB12 enriched by isotope ^{11}B [54].

From this thermo resist characteristic is seen that good operating interval for AIB12 based temperature sensors is between 150K-500K. The volt-ampere characteristic of the sample gives the opportunity of increasing the circuit sensitivity up to 10mV/grad over the whole temperature range. This sensor is characterized by high accuracy of the measurement, the error not exceeding 0.002.

The sensor can be designed as a miniature instrument for instantaneous responding to small temperature variation. It can be useful as a part of micromachines and all types of microsystems, which need the precise temperature measurements and works in hazardous conditions. It also can be applied to various areas of engineering, medicine, atomic power installations space power systems etc.

In latter case, if a ^{10}B isotope is replaced by the ^{11}B one; then such a microsystem can work in a radiation field without disturbing the structure with a sufficiently large fluency of neutrons. It is well known that thin films technology has a lot of specific advantages for sensor preparation.

At the same time it is a very powerful fabrication process for microsystems mainly because of very small volume involved in thin film sensors and extended surface, which helps to exhibit a strong reaction to their environment it may be, temperature, radiation or the partial pressure of a specific gas.

One more prospective application for boron based semi-conductor films is B₄C temperature sensors. At the fig.5 is shown the one simple variant of nuclear radiation-hardened B₄C temperature sensor enriched by ^{11}B [58].

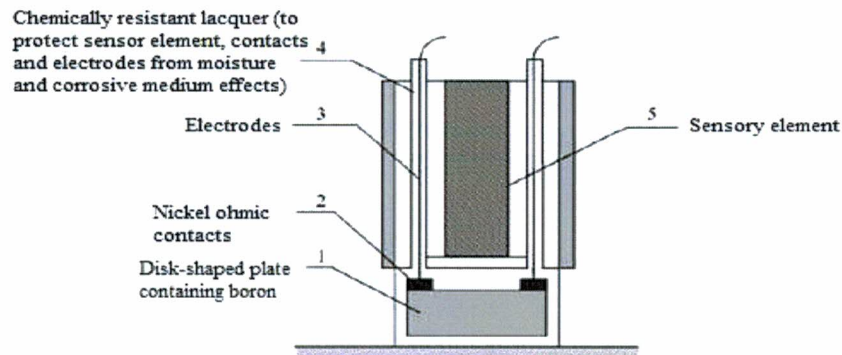


Figure 5. ^{11}B enriched B₄C sensory element based temperature microsensor [54].

QUANTUM EFFECTS IN NANOSTRUCTURES AND NANOSENSORS

Radiation sensors are systems that act as interfaces between incident radiation and imaging systems. The most effective way for organization of information transfer in these kinds of systems is quantum effects utilization. Recent study of the spin transfer in semiconductor nanosystems enriched by ferromagnetic dopants have determined the most essential mechanisms, responsible for spin transport properties, best solutions for electronic and magnetic structures preparation and for the development of technologies of spintronic materials with controlled disorders. Elaboration of precise methods of semiconductor nanostructures and systems preparation is extremely necessary for combination of well controlled spin electronic properties for semiconductors with additional possibilities of devices with the spin degree of freedom of current carriers. For this kind of quantum nanosensors it is the central problem today the search of an effective way for the spin injection in a semiconductor sensory element from the spin-polarized reservoir [59][60].

Generally, quantum sensors are devices those exploit quantum correlations to achieve a sensitivity or resolution that is better than can achieved using only classical systems can measure the effect of the quantum state of another system on it. The sensors operating with the tunnel magnetic junctions (MTJ) are the good example of spintronic quantum devices. There ferromagnetic electrodes are divided by very thin dielectric layer, and electrons are tunneling through a non-conducting barrier under influence of applied voltage [61].

Possibility of development of these sensory devices is connecting nowadays with the creation of spin transistors. Only in this case spintronic devices can not only switch or detect electrical and optical signals, but to enhance them and can be used as multifunction units.

Nanospinelectronics, based on usage of magnetic materials, represents new area of science and engineering. The reason to that is the perspective of creation of principally new devices for information technologies operating as charge, and spin degree of freedom of carriers, free from limitations inherent for metal spin electronic devices. The main structural property of materials in which we can observe novel nano dimension phenomena is their imperfection – high concentration of different defects connected with several impurities of metal and non-metal chemical elements. So, novel very exiting properties of semiconductors are determined by impurities and their disordered distribution. At the same time the last theoretical and experimental achievements have shown that disorders in semiconductors should be controlled – should have a necessary rules and regulations [62].

By these approaches, it is possible to define the link between matter and information which is most evidently manifested by the molecular constitution in building molecules connecting in given order. The initial formation directs the synthesis of sequences, which logically are not random; there is an optimization of structure within the system. Such optimization should be expressed in terms of fuzzy entropy and it relates directly to the definition of information. Following novel achievements we could integrate the science and technology of small scale structures (nano, pico structures) [63], quantum size elements based physical effects and information-communication processes, which brings us to novel applied science discipline – quantum information technology (QIT) [64].

The concept of spin injection and accumulation is based on induced magnetization in a nonmagnetic metal. However, this one description of spin injection and accumulation is only valid in the situation where a nonmagnetic metal is weakly coupled via tunnel barriers to its electrical environment [65].

The significance of spintronic is stipulated by perspectives of development and creation of new types of a non-volatile memory with random access (MRAM), quantum single-electron logical structures and ultra-dense information storage media. Thus, elementary information storage unit will be represented by an electron spin. The Giant Magneto Resistance effect (GMR) brightly has demonstrated, that a spin-polarized electrons can carry magnetic moment through non-magnetic materials with saving spin coherence, this is the meaning of the term “spin transport” nowadays (Figure 6) [66].

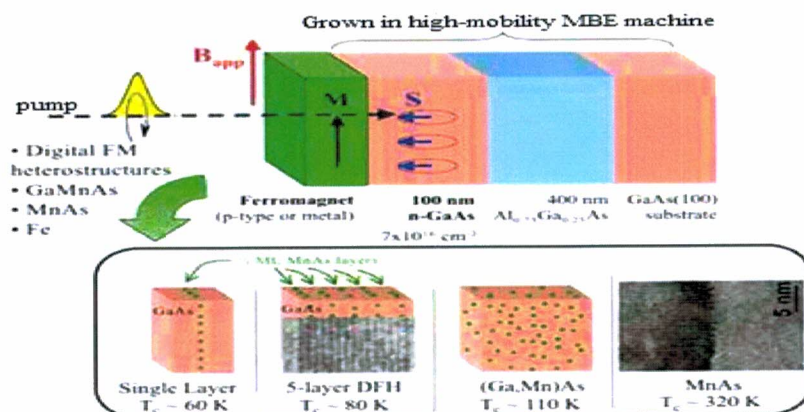


FIGURE 6. Electron spin coherence in ferromagnetic/gas nanostructures [66].

BONDING NATURE OF URANYL ION AND FUNCTIONALIZED GRAPHENE

With the cursory development of nuclear energy, radioactive wastewater has become of major concern and environmental challenge throughout the world. Uranium is one of the naturally occurred elements in nuclear energy programs. In the meanwhile, large amounts of uranium have been inevitably released into the environment and would cause serious health problems due to its extremely chemical and radioactive toxicity [67].

Hence, the removal of mobile uranyl ions from radioactive waste solutions is of great significance in terms of environmental protection and resource recovery. Adsorption approach has been considered to be of potential application for the separation of uranium from radioactive wastewater because it is high-efficient and easily handling.⁶⁸ In the past few years, the carbon materials such as activated carbon [69] carbon nanotubes (CNTs), [70-74] and graphene oxide (GO) [75-79] have been used as sorbents in elimination of uranium from radioactive solutions because of their large specific surface areas and strong adsorption abilities. Graphene has a planar-monolayer structure consisting of extraordinarily hexagonal sp²-bonded carbon rings. Therefore, it possesses many noteworthy physical and chemical properties such as high thermal conductivity, large surface area, and good thermal stability.⁸⁰⁻⁸³ In particular, graphene oxide containing abundant oxygen-bearing groups on the surface, which are much more hydrophilic than graphene itself, can efficiently bind metal ions through sharing an electron pair of the oxygen atom. Like other carbon materials in actinide pre concentration, the advantage of GO is that the adsorption and desorption of metal ions could be readily performed and GO itself can be fully incinerated, which is quite meaningful for the minimization of radioactive wastes. Therefore, GO has been considered to be an ideal supporting material for the removal of radionuclides from radioactive wastewater [78][84].

For instance, Wang et al. reported that GO showed excellent adsorption toward U(VI) and that the maximum adsorption capacity of U(VI) onto GO nanosheets was $97.5 \text{ mg} \cdot \text{g}^{-1}$ at 20°C .⁹ Later, an impressive maximum adsorption capacity of $299 \text{ mg} \cdot \text{g}^{-1}$ for U(VI) with single-layered GO was achieved by our group [76]. Very recently, a magnetic graphene/iron oxide composite was synthesized and used as a novel sorbent for U(VI) with high adsorption capacity of $69.49 \text{ mg} \cdot \text{g}^{-1}$ [77]. Although the adsorption of U(VI) with GO-based materials has been investigated experimentally, the structures of the uranyl/GO complexes and the corresponding thermodynamics properties are still not clear. Therefore, it is necessary to carry out theoretical investigation for better understanding the chemical behaviors of the uranyl ion with GO at the molecular level.

Several theoretical studies have been carried out on the adsorption of the uranyl ion onto organic molecules, carbon nanotubes, and fullerenes using quantum mechanical calculations based on density functional theory (DFT) [85-89]. Very recently, Kumar et al. has studied the uranium and plutonium complexes with G/GO to examine the applicability of a graphene-based fissile sensor using ab initio DFT method [90]. Moreover, the adsorption of uranyl ion onto various mineral surfaces have been investigated by both classical and quantum mechanical simulation techniques [91-96].

However, to the best of our knowledge, the adsorption of uranyl ion onto GO has still not been investigated theoretically. In the present work, to further understand the binding characters of uranyl ion onto GO, this study carried out the theoretical investigation on the interaction mechanisms between uranyl ion and GO using DFT method. The hydroxyl, carboxyl, and amido groups are the simple ligands that can efficiently bind toward uranyl ion [97–102]. Therefore, here we selected hydroxyl (–OH), carboxyl (–COOH), amido (–CONH₂), and dimethylformamide (–CONMe₂) as representative groups at the edge of the graphene to model and understand the bonding nature between uranyl ion and GO, which might help design new nanomaterials to efficiently remove radionuclides from radioactive wastewater.

Qun-Yan Wu *et al.* [103] were Studying the bonding nature of uranyl ion and graphene oxide (GO). This theoretical study is very important for understanding the mechanism of the removal of uranium from radioactive wastewater with GO-based materials. They are getting optimized [88] complexes between uranyl ion and GO applying density functional theory (DFT) combined with quasi-relativistic small core pseudo potentials. They studied oxygen-containing functional groups include hydroxyl, carboxyl, amido, and dimethylformamide. It is observed that the distances between uranium atoms and oxygen atoms of GO (U–O_G) are shorter in the anionic GO complexes (uranyl/GO^{-/2-}) compared to the neutral GO ones (uranyl/GO). The formation of hydrogen bonds in the uranyl/GO^{-/2-} complexes can enhance the binding ability of anionic GO toward uranyl ions. Furthermore, the thermodynamic calculations show that the changes of the Gibbs free energies in solution are relatively more negative for complexation reactions concerning the hydroxyl and carboxyl functionalized anionic GO complexes. Therefore, both the geometries and thermodynamic energies indicate that the binding abilities of uranyl ions toward GO modified by hydroxyl and carboxyl groups are much stronger compared to those by amido and dimethylformamide groups. This study can provide insights for designing new nanomaterials that can efficiently remove radionuclides from radioactive wastewater.

Binding Geometries for optimized [88] complexes formed between [UO₂(H₂O)₅]²⁺ and graphene where modified by oxygen-containing groups at B3LYP//ECP60MWB-SEG/6-31G(d) level of theory. The hydroxyl, carboxyl, amido, and dimethylformamide groups were selected to simulate the representative groups at the edge of GO. Moreover, the complexation strength of uranyl ion with a single monofunctional (M), ortho (OB)-, and meta (MB)-bifunctional GO have been compared. In addition, the neutral (at low pH) and anionic GO (deprotonated state at high pH) modified by hydroxyl and carboxyl groups are also considered. We labeled the anionic GO complexes as X'(A), X = M, OB, and MB, and A = –OH and –COOH as shown in Figures 7 and 8, respectively. For the amino and dimethylformamide functionalized GO complexes, the uranyl ion coordinated to the oxygen atom are labeled as M(B), OB(B), and MB(B), B = –CONH₂ and –CONMe₂, while the uranyl ion coordinated to the nitrogen atom are labeled as M'(B), OB'(B), and MB'(B), B = –CONH₂ and –CONMe₂ as shown in Figures 9 and 10.

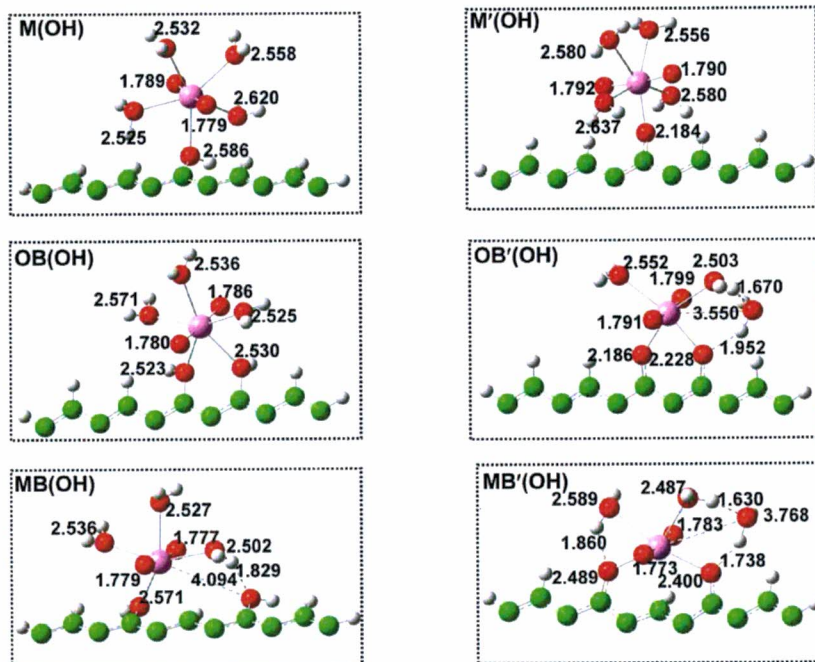


FIGURE 7. Uranyl/G(OH) complexes optimized structures using the B3LYP method. The representative structural parameters are labeled in the snapshots [103].

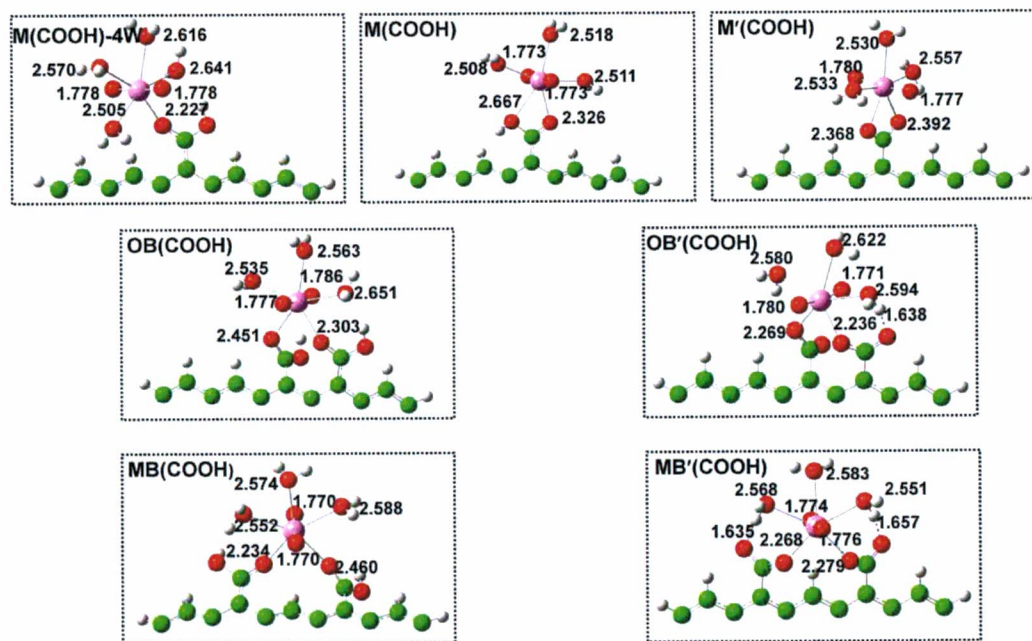


FIGURE 8. Structures of the uranyl/G(COOH) complexes optimized using the B3LYP method. The representative structural parameters are labeled in the snapshots [103].

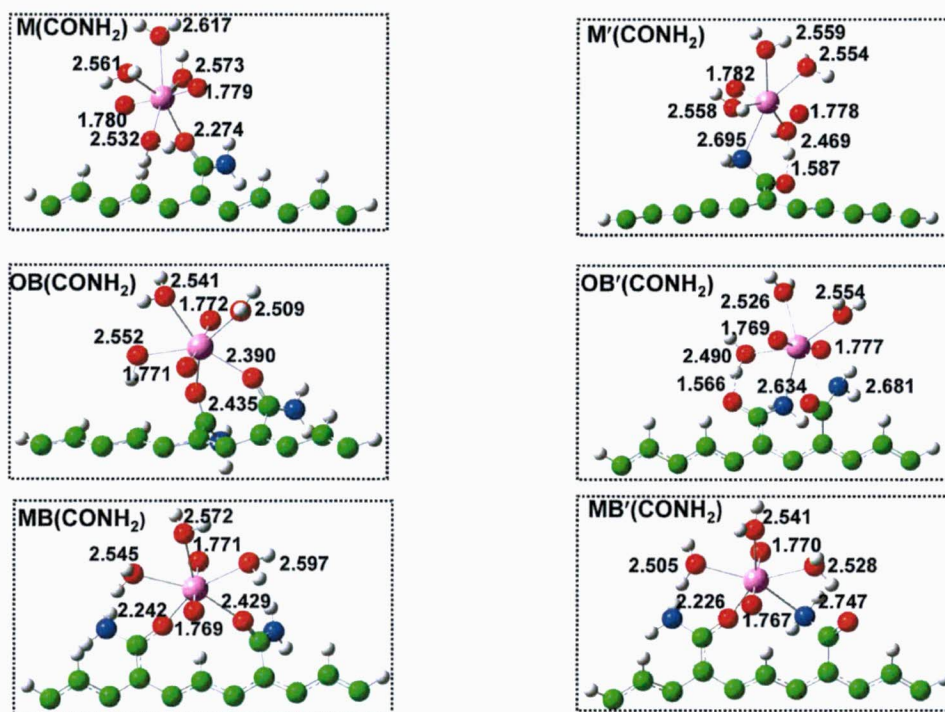


FIGURE 9. Uranyl/G(CONH₂) complexes optimized structures using the B3LYP method. The representative structural parameters are labeled in the snapshots [103].

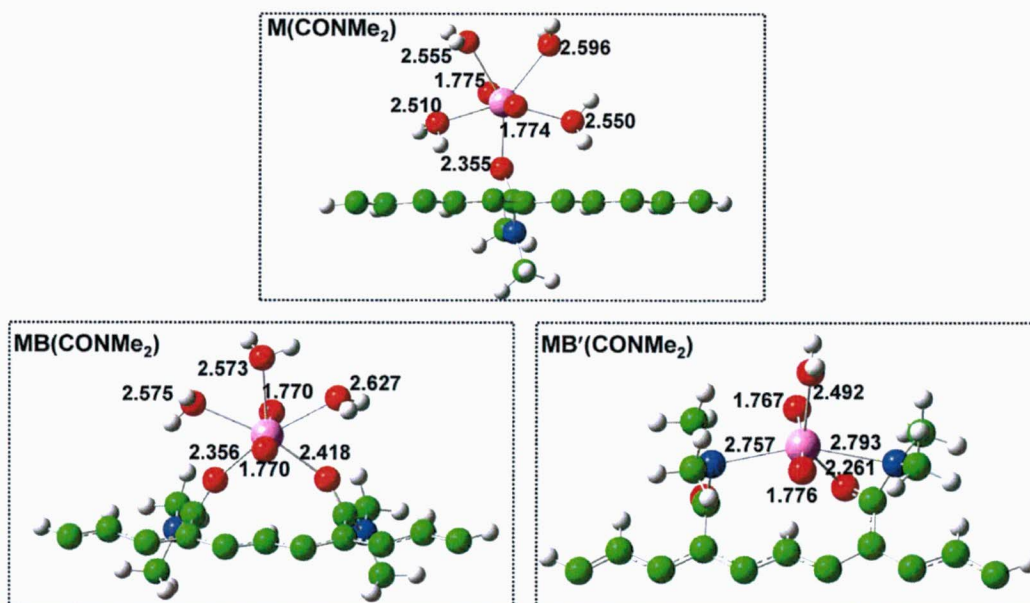


FIGURE 10. Uranyl/G(CONMe₂) complexes optimized structures using the B3LYP method. The representative structural parameters are labeled in the snapshots [103].

CONCLUSION

Through what has been put forward in this publication of studies of the evolution of the work of nanosensors, we conclude that all of the studies that have achieved results in the areas of nanosensors will lead later to get to deal with the scale of less than nanotechnology and perhaps we will see during

the subsequent years, studies proceed to pico-technology will be another revolution in the field of nuclear sensors and dealing with ionizing materials and detection, especially those concerning methods nuclear waste water

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