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Molecular Interactions and Spectral Changes of Beta-and Gamma-Irradiated Silicon Clusters with different Time Intervals

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Abstract: : Silicon clusters have garnered significant interest due to their unique physical and chemical properties, which make them valuable in fields such as nanotechnology, optoelectronics, and materials science. The purpose of this research is to investigate the effects of beta and gamma irradiation on silicon clusters, with a particular emphasis on gaining a knowledge of how irradiation over varying time intervals contributes to the molecular interactions and spectral features of silicon clusters. The ambient pressure and the two-step acid-base catalysis were both reliant on the manufacturing process. Beta and gamma radiation were used as sources at 2, 4, and 6 hours. The work combines spectroscopic analysis with molecular interaction assessments, and it makes use of FTIR analysis, N2 adsorption-desorption, FESEM, and EDS in order to shed light on the behavior of silicon before and after it has been irradiated in varied concentration clusters across time. Based on the findings, it was determined that the samples that were subjected to gamma radiation did not exhibit any discernible changes in their chemical structure, pore structure, or even surface appearance. Beta irradiation was applied to the samples for a period of six hours, and after that, there was a small alteration in the pore structure of the sample, the surface area decreases from 851.02 before irradiation to 833.03 at Beta Rad. This decrease occurred due to gamma radiation. The reduction was minimal. After irradiation, the pore size decreases from 10.44 to 0.9 and 0.8, while the pore volume, particle size, and pore diameter increase*.* The FE-SEM images show morphological stability; indicates that its unique porous nanostructure remains largely unaffected under radiative stress. The study comes to the conclusion that silica aerogel is a material that has the potential to be used in radiation isolation.

Keywords: Silica Aerogel, Beta, Gamma, Surface Area, FTIR, Molecular

1. Introduction

The technology of manufacturing radiation-resistant materials is one of the promising technologies, because of its importance in many applications [1, 2]. For example, their use in the preservation of radioactive materials, radiation-protective wall coatings [3]. it can also be used in the manufacture of clothing or masks and hats to protect from dangerous radiation [4] From this point of view, attention was paid to the manufacture of materials with high tolerance to harmful radiation, taking into account the low cost and quality [5, 6] such as materials made of polymers, optical fibers or radiation-resistant glass [7, 8], especially Glass made of silica gel, within special specifications [9,10]. Since ancient times, silica gel has attracted the attention of researchers because it has many distinctive characteristics, such as low density, low thermal conductivity, a high surface area, as well as good transparency [11, 12] All these properties are due to the fact that most of its components are air, as air makes up more than 90 percent of its components and the rest are silica nan-network[13] and it was found that these specifications do not change even if silica is grafted with laser dyes or metal ions if it maintains being nanoparticles with a high surface area and a homogeneous morphological composition [14,15]. The researchers have conducted much research that has proven the amazing properties of silica gel and it has also succeeded in many scientific and industrial applications such as crude oil adsorption, self-cleaning windows, drug delivery and other applications [8, 16, 17]. Ionizing radiation is of significant interest to several researchers, since it has sufficient energy to displace tightly bonded electrons from atoms, so generating ions (charged particles). Numerous research has examined the impact of this radiation on several materials, including aerogel. The capacity to efficiently identify and protect against ionizing radiation is crucial in several settings, including nuclear power facilities, medical imaging, and space exploration. Subsequent lines will delineate investigations about ionizing radiation and its association with aerogel [18, 19]. Jingyi Xie and others study the Impact of γ-radiation on silica aerogel and composite substances for thermal rinsulation usage in nuclear energy pipelines, they found at the radiation of 1700 kGy thermal conductivity increased by 30 %, Silica aerogel demonstrated exceptional structural stability [20]. GW Mohammed and others exposed to Cs-137 at different times and investigate the effect of irradiation on samples, The results indicated slight changes in the molecular structure of the samples[21]. Also D.L. Perego exposed his samples to intense (proton, neutron, and gamma) radiation, to humid air and C_4F_{10}. The results shown no changes in the optical and structural properties [22]. While Tatsuya Ito and others separated of Cs(I) from HNO_3 solution then exposed with A microporous silica-based (Calix[4]+Dodecanol)/SiO_2, they found that the adsorption of Cs(I) by the adsorbent in a gamma-ray field exhibited characteristics comparable to those of adsorption without irradiation up to a minimum of 170 kGy [23]. Also, Elchin M. Huseynov study the effect of gamma irradiation on Zr-C nanoparticles, and founds that the peaks corresponding to Zr_ O become more acute as a result of gamma radiation and more amorphous structure [24]. While Elchin Huseynov and others, analyzed the FTIR spectrum for SiO2 before and after gamma irradiation, they found from absorption spectrum five new peaks appeared two of them were influence gamma radiation [25]. Besides the same others make examination of the spectral properties of TiC samples when exposed to gamma rays. they found that a group of bonds disappeared due to gamma rays, while maintaining the homogeneous structure [26]. In this work the low-density silica gel samples were exposed to beta and Gamma radiation; the exposure was carried out at a constant energy and with time intervals starting from 2, 4 to 6 hours. This work focuses on the effects of beta and gamma irradiation on silicon clusters, with an emphasis on understanding how irradiation over different time intervals influences their molecular interactions and spectral characteristics. Irradiation is known to induce structural modifications, electronic state transitions, and potential defects within clusters, which can alter their optical and electronic properties. By investigating these changes, we aim to explore the mechanisms of radiation-induced effects and their implications for advanced material design and radiation-resistant applications. This study combines spectroscopic analysis with molecular interaction evaluations to shed light on the behavior of irradiated silicon clusters over time.

2. Materials and Methodology

Simarouba seeds were first processed using an automated moisture reduction system to achieve appropriate drying conditions, followed by a hybrid peeling mechanism that combined individuals and mechanical shelling for maximum efficiency. The kernels were then processed through a high-pressure mechanical expeller with automated temperature and pressure controls to obtain high-purity Simarouba oil. The extracted oil, seen in Figure 1, was utilized as the base feedstock for biodiesel manufacturing. Simarouba oil was converted into Simarouba methyl ester (SME) through a transesterification method. The reaction system included a 2-liter, three-necked round-bottom flask equipped with a high-torque magnetic stirrer and a temperature-controlled heating mantle for precision thermal management. A closed-loop control system was used to adjust the methanol-to-oil ratio and optimize reaction conditions. Methanol was employed in excess as the alcohol, while potassium hydroxide (KOH) served as a homogeneous catalyst.

2. Materials and Methods

2.1 Materials

Tetraethylorthosilicat (TEOS), trimethylchlorosilane (TMOS), from sigma Aldridge, n-Hexane with a purity of > 98% CHem-LAB (Belgium) Ethanol, ammonium solution, ammonium fluoride, Hydrochloride Acid solution Thoma Baker (India), Deionized water was lab-made.

2.2 Preparation and characterizations

Ambient pressure and two-phase acid-base catalysis factor the method implemented in the preparation of samples where the molar ratio of each [TEOS: Etho: HCl] were [1.5:5.5:0.2] respectively. Acid-base catalysis is an effective method for preparing silica aerogel samples, as it produces a homogeneous structure. The acidic medium delays the gelation process, allowing for the formation of a long silica network. This is known as the hydrogenation stage. In the second stage, the addition of the base, the silicon molecules begin to come closer together, forming what is known as condensed silica, which later turns into a gel. The pH can also be controlled using this type of catalysis [27]pH for all samples fixed at 8 where a good percentage of the sol turns into a gel in a short time ranging from 10 to 15 minutes. After converted to gel, the aging time in ethanol was 30 min, then wash three times in pure hexane and immersed the alcogel in solution consist of TMCS + n-hexane in percentage ration 1:6 under 60˚c for 8hr., in order to surface modification. The modified gel washed in n-hexane two times and let them to dry at room temperature.

2.3 Radiation Methodology

All samples were divided into two equal-weight sections to ensure consistency in radiation exposure and subsequent analysis.

Each section was exposed to ionizing radiation using pre-calibrated beta and gamma sources, The experiments were conducted at room temperature (approximately 22 ± 1°C) within a lead-shielded irradiation chamber to eliminate background radiation effects. Beta radiation was provided by a Strontium-90 (Sr-90) source, while gamma radiation was supplied using a Cobalt-60 (Co-60) source as shown in table (1) [28]. Samples were positioned at a standardized distance from the radiation source to ensure uniform dose distribution, Exposure durations were set at 2, 4, and 6 hours, with each sample irradiated separately to avoid cross-contamination. Prior to experimentation, both beta and gamma sources were calibrated using a traceable ionization chamber certified by a national metrology institute. The Average dose rates were: beta ~0.25 Gy/h, gamma ~0.40 Gy/h were determined by Chemiluminescent dosimeters (TLDs) were placed adjacent to each sample.

Table 1. Some information of beta and gamma sources

source	Beta	Gamma
Decay Energy MeV	0.317	1.173
sample	^{60}Co	^{60}Co
Half-life time ($t_{1/2}$)	28.79 years	30.18 years
Isotopes mass	89.907Da	59.933Da

All samples are divided into two equal weight sections and exposed to beta and gamma sources for 2, 4, and 6 hours. The FTIR analysis "Bruker FTIR Spectrometer ALPHA II, USA within the 400–4000 cm^{-1} "was used to find out about the compositional properties of the molecular bonding before and after irradiation, while A high-resolution FE-SEM model (MIRA3 TESCAN) used to study the surface features. Also, determine their specific surface area and pore size distribution. The BET technique or nitrogen adsorption desorption employs non-corrosive gases (such as nitrogen) as adsorbates (BELSORP-mini II).

3. Results and Discussion

3.1 FTIR analysis

Fourier-transform infrared (FTIR) spectroscopy is a powerful technique to characterize materials by identifying their functional groups based on specific absorption bands. Several distinct bands are observed for silica aerogel, each corresponding to different vibrational modes. Figure (1) shown the changing in FTIR spectrum before and after irradiation with Beta sources. It's clear that the broad bands at 3423 cm-1 and weak band at 1234 cm-1 corresponds to the O-H stretching and Si-OH [10, 29], enhancing the sample hydrophobicity lead to weaking the bands in the prepared samples. the strong peaks at 1076 and 852 cm-1 attribute to the vibration and stretching of Si–O–Si and Si-O respectively, while the band at 3820, 2966, and 655 cm-1 refer to C-H stretch and asymmetric of CH2 and C-H respectively [30, 31], these peaks are appeared as a result of surface modification with silane groups. Through the analysis of FTIR, it found that the effect before and after irradiation was slight and did not significantly affect the molecular bonding of silica samples even when irradiated for 6 hours, which indicates that silica gel pneumatic can resist Beta and gamma radiations for a long period without changes in the structure, which may be attributed to the high porosity enjoyed by silica aerogel. Figure (2) refer the FTIR spectrum in case of Gamma irradiation.

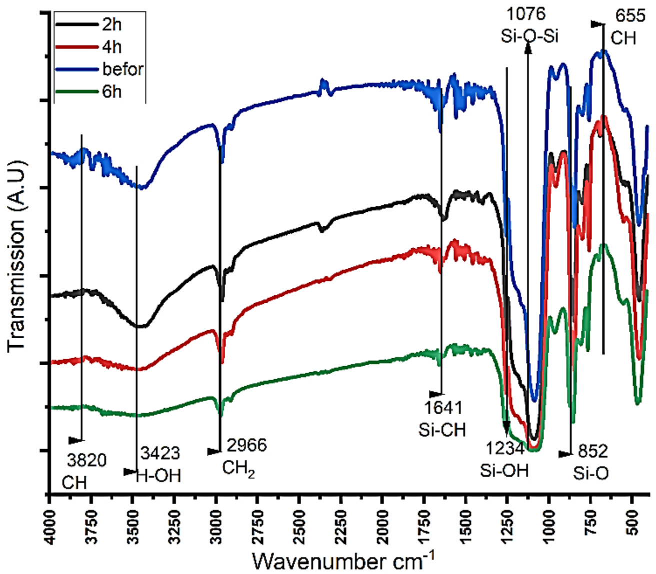

Figure 1. FTIR analysis for silica Silicon clusters before and after beta irradiation with different time intervals

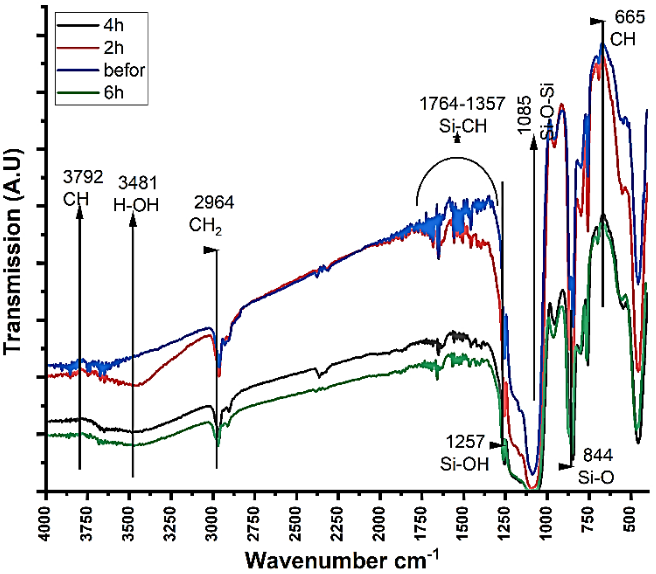

Figure 2. FTIR analysis for silica Silicon clusters before and after gamma irradiation with different time intervals.

The molecular structure of silica gel did not show a noticeable change in the FTIR spectrum upon irradiation with Gamma for the longest selected period of 6 hours. As in Figure 1, it finds that the bond positions of both CH, CH2, and Si-O almost remained the same while the bands Si-CH, H-OH, and Si-OH have changed in their positions, in these regions may be that the absorption of radiation by the hydroxide groups occurred, which led to a change in the wavenumber. But this is not of great importance when talking about compositional changes due to irradiation. Generally, the effect of beta irradiation more than gamma, because Gamma rays are lost immediately after hitting matter, while beta rays are lost gradually. This makes beta rays better able to penetrate and interact with matter, enhancing their effect more than gamma rays. However, it can be said that the molecular structure and the binding sites did not experience significant changes when irradiated with beta and gamma starting from 2 to 6 hours. This is why we are seriously thinking about the possibility of silica gel to counteract beta and gamma rays and the possibility of using it as a radiation-insulating material.

3.2. Nitrogen adsorption-desorption

Hysteresis loop shapes often enable the identification of the pores types and classification system for physisorption isotherms, indicating specific types of pore connectivity and blocking.

Figures (3 a, b, and c) show the results of Brunauer-Emmett-Teller (BET) analysis, represented by N2 desorption-adsorption hysteresis loops of silica aerogel before and after irradiation with Beta and Gamma radiation. Also, the change in pure dimeter mapping (MP) and pure size distribution (BJH) are shown in figures (4). The utmost volume of pore size can be classified as Mesopores type, where most of the pore sizes within the range below 20 nm diameter are mixed with some Micropores with dimension between 2-3 nm. Mesopores are commonly present in materials such as silica gels, surface aera results refers to that the nano-property is domain before and after irradiation, also, no change in specific surface as a result of radiation except of some variations in the particle size and pore size, volume and dimension. From figures 3, it can say that the loop type affects calculations of surface area and porosity, which are crucial for catalysis, adsorption, and filtration applications [32, 33]. Both adsorption and desorption branches loop appear as gradual variations with the variation of relative pressure, which is classified as H3 type. The H3 loop is usually associated with materials that have slit-shaped pores. The H3 loop indicates that the pores are not closed, suggesting that the material has open, accessible pores that allow for continuous adsorption and desorption without significant pore blocking [34, 35]. The material transitions from H2 hysteresis loops to an H3 loop, which suggests a change in the pore structure from ink-bottle or complex network pores to more slit-like pores [36]. This conversion is due to changes exposed with radiation, these properties remain largely constant in aerogel silica due to the stability of the product and its resistance to external conditions such as heat (less than 500 degrees) and high pressure. When silicone formations exhibit high porosity, a big surface area, tiny particle size, and a distinct pore size, they become much more important. The significance of each is further upon here: The presence of many particles that contribute to practical applications like medication administration or oil adsorption is indicated by a high porosity, which is an indicative of a large surface area. The surface area grows as the particle size decreases. Conversely, if the silica network is porous, it signifies that it has big spaces. This study's findings suggest that the presence of air in these spaces significantly increases their thermal insulation capacity and, by extension, their resistance to radiation impacts. These interesting properties were obtained even when the samples were exposed to Beta and gamma radiation for a maximum of 6 hours. From the figures, it notices that the samples retained the following properties: surface area, pore volume, and pore dimensions, with slight changes as shown in Table 2. It was noted that there were noticeable changes in the shape of the hysteresis rings before and after irradiation, these effects also appeared (MP) and BJH-plot (figure 4), these changes can be classified as physical if they do not fundamentally affect the structural properties of the samples. Therefore, it was necessary to resort to the FTIR test, which proved the validity of the above statement.

Table 2. BET physical properties before and after beta and gamma irradiation

	Before rad.	Beta rad.	*gamma Rad.*
BET Surface area (m^2/g)	851.02	833.03	840.11
Pure size (nm)	10.44	0.9	0.88
Pure volume (nm)	2.22	3.3315	3.02
Ave. pure dimeter (nm)	15.90	17.018	17.32
BJH average pore width (nm)	1.012	1.22	1.37
Average Particle Size (nm)	22.23	26.60	24.1

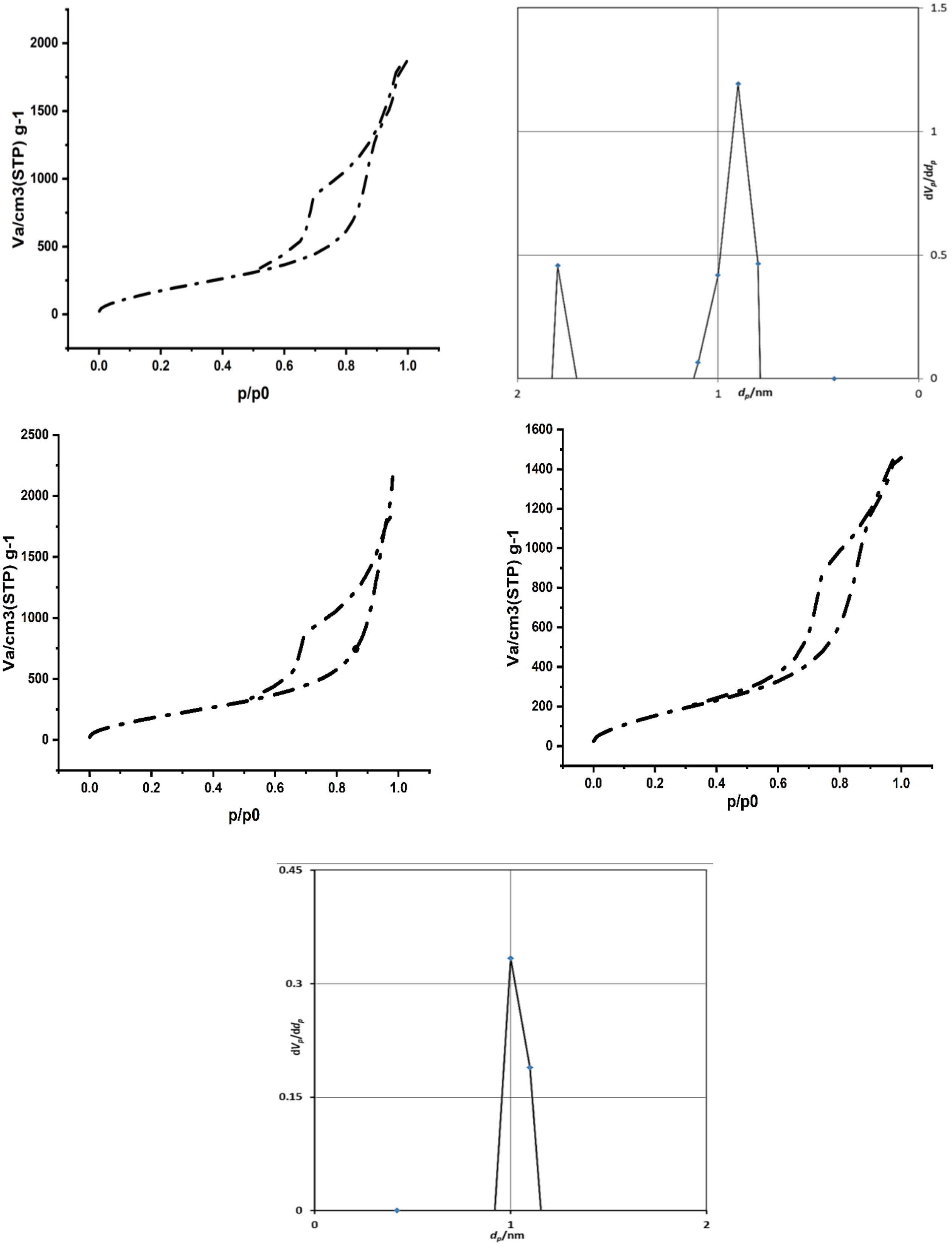

Figure 3. N2-adsorption-desorption for silicon clusters (a) before and after (b) beta (c) gamma irradiation.

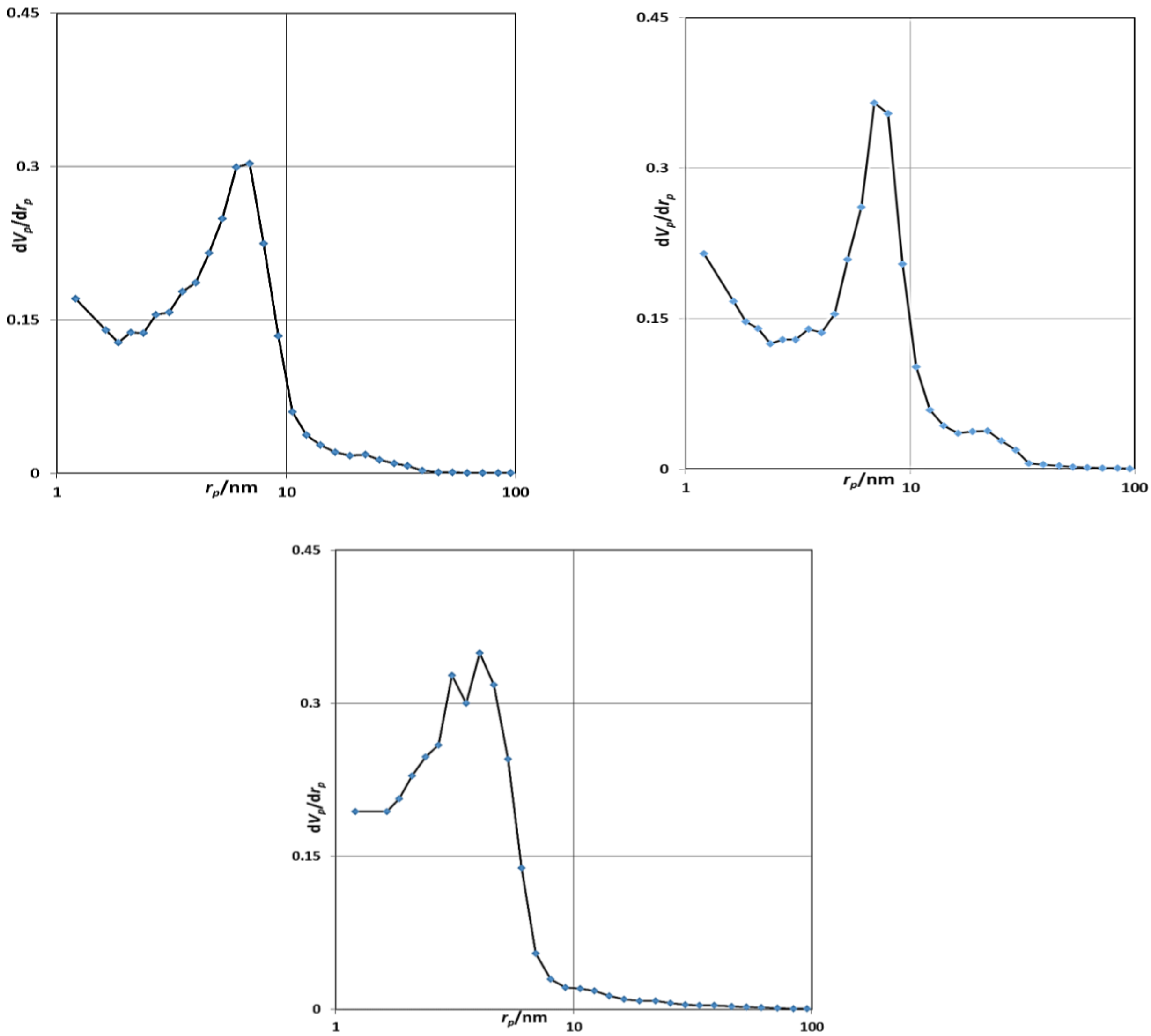

Figure. 4. BJH plot for silicon clusters before and after beta and gamma irradiation

3.3. Field-Emission Scanning Electron Microscopy Analysis

Figure (5) show the FE-SEM images for silica monolith before and after exposed with beta and gamma irradiation. Different magnifications were shown and presented a generally homogeneous structure with small spherical-like particles, no large aggregates forming the entire silica structure. There are some mesopores between the attached nanoparticles. When comparing the shapes before and after irradiation we find that there are no significant changes in the surface morphology, the silica aerogel appeared clustered, and the particles not packed together or aggregated with a smooth surface. Also, the variation in surface behavior resulting from incorporating large organic molecules caused alteration of the surface with trimethyl groups and reversible shrinkage in the wet gel silica after drying. These variations in pore behavior may induce variation in the entire pore shapes and their connectivity.

Figure (6) presents the EDX spectra for the three samples. The EDX analysis confirmed the presence of Si and O elements; the C element as a residual comes from the started solvent, The high content of the O element is attributed to adsorbed oxygen species present on the nano-surface. No additional peaks appeared in all samples, indicating the purity of the prepared samples. There do not appear to be significant changes in the proportions of the basic element's silicon, oxygen and carbon before and after irradiation, which indicates that there was no reaction, fusion or even a change in the composition of the basic elements that make up the silica aerogel.

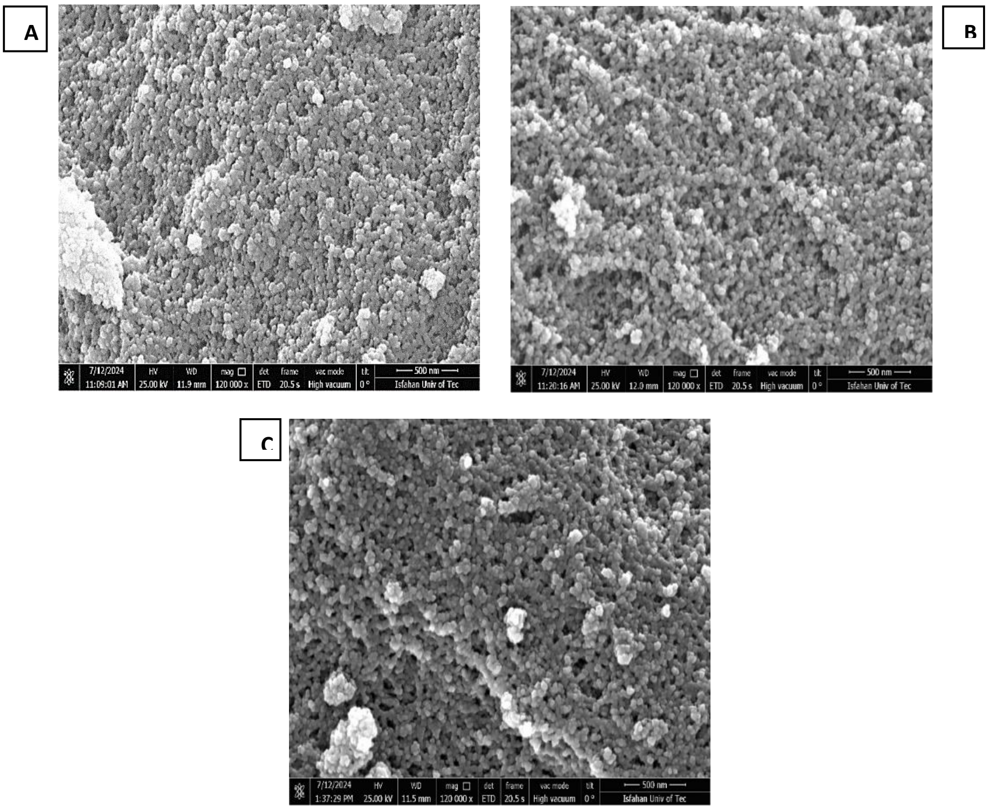

Figure. 5. FE-SEM images for silica monolith (A)before and after exposed with (B)beta and (C)gamma irradiation.

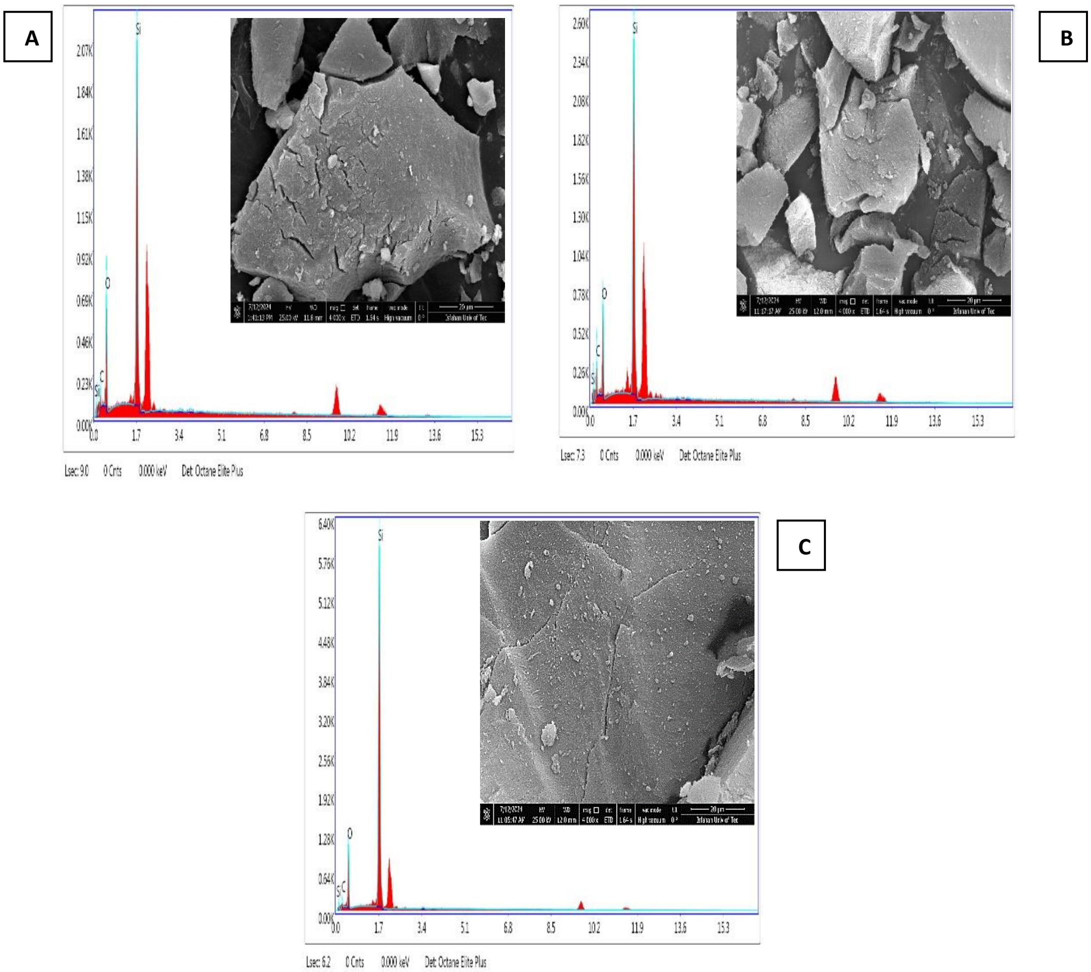

Figure 6. FESEM images and EDX analysis for silicon clusters (A) before after (B)beta and (C) gamma irradiation

The SEM results refers to the morphological stability of silica aerogel following exposure to ionizing radiation indicates that its unique porous nanostructure remains largely unaffected under radiative stress. This has several critical implications for its long-term stability and suitability in radiation-rich environments for example the preservation of Porosity and surface Area whereas silica aerogels are valued for their extremely high surface area and open pore network. Morphological stability implies that radiation does not significantly collapse or shrink the porous structure, ensuring that key functional properties — such as low density, thermal insulation, or adsorption capacity — are retained over time.

4. Conclusions

The high porosity and specific surface area played an important role in enabling the silica gel to resist beta and gamma radiation for up to 6 hours of exposure. Upon examining the characteristics before and after irradiation, we discovered that the surface morphology remained unchanged, the silica remained monolithic, and the particles lacked packing or aggregation with a smooth surface. Additionally, the incorporation of large organic molecules resulted in a variation in surface behavior, which altered the surface with trimethyl groups and caused reversible shrinkage in the wet gel silica after drying. Also, the molecular structure of silica gel did not show a noticeable change in the FTIR spectrum upon irradiation with gamma for the longest selected period of 6 hours. also, silica aerogel's morphological stability under radiation confirms its resilience and extends its applicability to advanced technological domains where radiation resistance is a critical material requirement. This is why we are seriously considering the use of silica gel as a radiation-insulating material to counteract beta and gamma rays.

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Authors Contribution Statement

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Competing Interests

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