Electrostatic Properties and Mulliken Atomic Charge Analysis of Stability for Nanoscale SiO_2 Ring Clusters: Density Functional Theory

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Abstract: Ring clusters of SiO_2 nanoscale have attracted attention for applications in a variety of fields, including electronics, optics, and catalysis. To properly construct and operate these clusters, one must understand how they respond and maintain stability. This study investigated the stability of nanoscale SiO_2 ring clusters with various planar folds using calculations based on density functional theory (DFT), analysis of potential molecular electrostatic potential (MEP), and Mulliken's atomic charge. Our results show that the silicon atoms in the clusters are significantly electrophilic, but the oxygen atoms are substantially nucleophilic. Polarization and stability levels are seen in the regions between silicon and oxygen. The symmetry and stability are affected by their planar fold, which also affects the patterns of electrostatic potential and charge distribution. Understanding the stability of nanoscale SiO_2 ring clusters, as demonstrated in this work, may contribute to the development of novel materials tailored for specific applications. By improving our understanding of the stability of SiO_2 ring clusters, we can design them more effectively for a variety of applications in fields such as electronics, optics, and catalysis. This will contribute to the growing body of knowledge on the characteristics and behaviors of nanoscale materials where stability is critical**.**

Keywords: **SiO_2 ring clusters, density functional theory, electrostatic potential energy maps, stability, Mulliken atomic charges.**

1. INTRODUCTION

The SiO_2 ring clusters offer several advantages [1–3]. First, SiO_2 optical waveguide ring resonators (OWRR) with high Q and mode selectivity can be used to achieve single-mode oscillation in an optoelectronic oscillator (OEO) and improve the performance of microwave signals [4]. Additionally, SiO_2 nanoparticle clusters serve effectively as catalyst excipients, improving the dispersion of active metals and preventing metal sintering during processing and catalysis [4]. SiO2 ring clusters also have the potential for bottom-up synthesis, since the (SiO_2) cluster exhibits a highly uniform structure making it a potential building block for the development of crystalline nanoporous materials [5]. In long-wavelength InAs / GaSb type II infrared superlattice photodiodes, the SiO_2 composite passivation process improves the surface deep current and surface resistivity, resulting in stable and efficient passivation [6]. In the development of the lithium metal battery based on the LVP cathode, the hybrid solid-state electrolyte and mesoporous SiO_2 scaffold reveals high ionic conductivity, wide electrochemical window, good compatibility with cathode material f, which can hold its lithium dendrites for blocking [7]. In general, SiO_2 ring clusters provide significant advantages across optoelectronics, catalysis, and materials science. SiO_2 nanoparticles have received considerable attention due to their great potential in system design for filtration, separation, drug delivery, optics, electronics, and catalysis [8]. Ring formation and breakage during silica polymerization can occur more rapidly in dilute systems, leading to dense aggregates, whereas slower reorganization in concentrated systems preserves random branched structures [9].

Electrostatic potential energy maps of nanoscale SiO_2 ring clusters can be used to predict their stability by using density functional theory (DFT) [10]. DFT analysis allows for the calculation of charge states, bond lengths, and total energies of clusters, providing valuable information about their electronic structure [11]. By examining electrostatic potential energy maps, one can gain insight into the distribution of charge and the strength of chemical interactions within the clusters [12–16]. This information can then be used to assess the stability of the clusters and predict their stability [17]. Furthermore, DFT calculations can provide data on cluster geometries, stabilities, and electronic properties, such as binding energy, fragmentation energy, and HOMO-LUMO gap, which further contribute to understanding their stability [18–21]. Overall, the integration of DFT calculations and analysis of electrostatic potential energy maps provides a powerful approach to studying the stability of nanoscale SiO_2 ring clusters.

The calculation of atomic charges of Mulliken plays a crucial role in the application of quantum physical and chemical calculations to molecular systems because atomic

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charges affect the dipole moment, molecular polarizability, electronic structure, and many properties of molecular systems [22–26]. The relationship between Mulliken atomic charges with different planar folds in SiO_2 nanoring clusters and their interaction has not been directly addressed in previous research works. However, the abstracts do discuss the electronic structures of various silicon clusters. For example, Donoso-Tauda et al. found that the transition from planar structures to three-dimensional structures increases and decreases polarizability [27]. Gong observed that the dangling bonds of Si clusters can be stabilized by superatoms, leading to kinetic stability [28]. Kaxiras proposed that intermediate-sized Si clusters with all surface atoms participating in reconstructions are stable due to covalent bonding [29]. While these results provide insight into the stability of silicon clusters, the specific relationship between Mulliken atomic charges and stability in SiO_2 ring clusters has not been addressed in previous work. In this work, we aim to investigate this relationship directly.

In this paper, we investigate the steadiness and stability of nanoscale SiO_2 ring clusters with unique planar folds using density practical theory (DFT), molecular electrostatic capacity molecular electrostatic potential (MEP) evaluation, and Mulliken atomic fee calculation. We have found that the oxygen atoms are the most nucleophilic, and the silicon atoms are the most electrophilic inside the clusters and that the regions between them are the highest polarized and reactive. We also determined that the planar fold influences the symmetry, balance, and stability of the clusters as it affects the fee distribution and electrostatic ability patterns at the molecular surface. Our results provide valuable insights into the structural balance of nanoscale SiO_2 ring clusters and may contribute to the layout and development of novel substances with desired properties.

2. METHODOLOGY

The technique employed in this observation forms the basis for examining price transfer or conjugative interactions in distinct planar folds in nanoscale SiO_2 ring clusters and to discover its electrophilic and nucleophilic sites, Mulliken population analysis (MPA) and the surface of the molecular electrostatic capacity or molecular electrostatic potential (MEP) of the title molecule have been studied using the density functional theory (DFT). These computational strategies have been chosen for their established accuracy and effectiveness in characterizing the price distribution and electrostatic homes of molecular structures. The following steps define the distinct processes carried out in this research:

2.1. SYSTEM PREPARATION

The SiO_2 ring clusters with one-of-a-kind planar folds (starting from 2-fold to eight-fold) have been selected as the subjects of this study in Figure 1(a), (b), (c), (d), (e), (f) and (g), respectively. These clusters exhibit versions in their structural preparations, impacting their electronic homes and stability.

2.2. GEOMETRY OPTIMIZATION

The initial atomic coordinates of the SiO_2 ring clusters were installed. Subsequently, geometry optimization changed into executing the use of the DFT method. The B3LYP purposeful and the 6-311G (d) basis set were used for the optimization method. The B3LYP functional

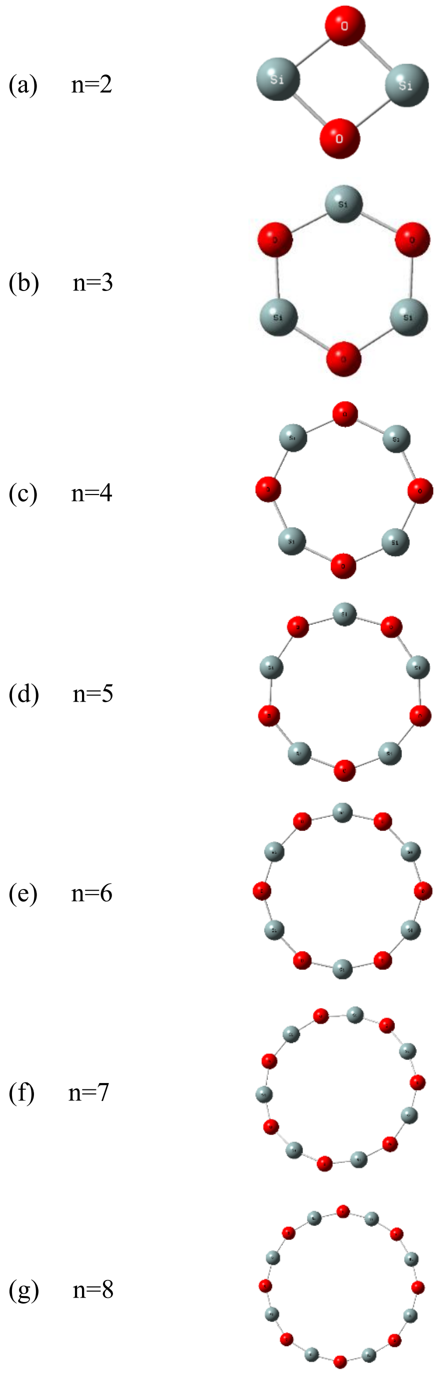


Fig. 1. The figure shows the molecular structure of nanoscale n-fold SiO_2 ring groups, indicated as (a), (b), (c), (d), (e), (f) and (g) for values of n equal to 2, 3, 4, 5, 6, 7, and 8, respectively.

combined with the 6-311G (d) basis set was chosen for the geometry optimization of SiO_2 ring clusters due to its effective balance between accuracy and computational efficiency according to Zhao et al. work [35]. The hybrid functional exhibits limitations when quantifying strong electron correlations alongside weak dispersion effects, since it requires supplemental correction mechanisms [36]. Constraints affecting the SiO_2 ring clusters do not significantly impact the research results of this study. Geometry optimization ensures that the molecular systems represent strength minima, yielding strong and dependable starting points for subsequent calculations.

2.3. DENSITY FUNCTIONAL THEORY CALCULATION

The core of this research is based on the application of density functional theory (DFT). DFT calculations were performed using the Gaussian 09 and GaussView05 software packages [31]. The DFT / B3LYP calculations generated essential facts, such as digital energies, electron density distributions, and atomic coordinates, which can be pivotal for the investigation of electrostatic homes [32–35].

2.4. MOLECULAR ELECTROSTATIC POTENTIAL (MEP) CALCULATIONS

The molecular electrostatic potential (MEP) calculations were performed postgeometry optimization as well as the DFT calculations. The primary objective was to visualize the electrostatic potential on the surfaces of the SiO_2 ring clusters. The MEP is a scalar field representing the electrostatic potential at different spatial locations around the molecular system. It indicates how a positive test charge would interact with the molecular charge distribution at a given point. MEP calculations facilitate the identification of regions with high electron density (displayed in red, indicating negative potential) and regions with low electron density (displayed in blue, indicating positive potential) on the molecular surface. The GaussView05 program was used to visualize and interpret the MEP energy maps, providing a visual representation of the electrostatic potential values.

2.5. MULLIKEN ATOMIC CHARGE CALCULATION

The Mulliken atomic-fee calculations were performed as part of the DFT calculations. These calculations decide the atomic fees in the SiO_2 ring clusters. Atomic costs are essential for understanding the distribution of electrons and the number of atoms within the clusters. They contribute to various molecular properties such as dipole moment, polarizability, and stability. The Mulliken atomic fee analysis proved instrumental in identifying regions within the clusters where atoms exhibited electron-rich (negatively charged) or electron-deficient (positively charged) conduct.

The detailed methodology above ensures accurate characterization of the charge distribution and electrostatic behavior of nanoscale SiO_2 ring clusters with different planar folds These computational methods provide a solid foundation for understanding cluster behavior and catalytic content. It has wide applications in fields such as science, nanotechnology, etc. The combination of DFT calculations, MEP analysis, and Mulliken atomic charge determination provides a comprehensive view of the electronic properties and stability patterns of these nanoscale structures.

3. RESULTS AND DISCUSSIONS

The molecular electrostatic potential (MEP) is a valuable tool for studying stability, given that an approaching electrophile will be attracted to negative regions (the electron distribution where the effect is dominant). In the majority of MEPs, the regions of maximum negative potential, indicated in red, correspond to preferred sites for electrophilic attack, while regions of maximum positive potential, shown in blue, indicate preferred sites for nucleophilic attack. The importance of MEP lies in its ability to simultaneously display the size and shape, along with positive, negative and neutral electrostatic potential regions in terms of colour grading. This makes it a valuable tool for studying the relationship between molecular structure and physiochemical properties [55]. The outcome is a single display of both the molecule size and the electrostatic potential value. Here, 3D plots of MEPs of the SiO_2 ring groups with distinct planar folds are presented in Figure 2. The MEP is an electrostatic potential mapped onto the constant electron density surface. Different colours represent various values of the electrostatic potential on the surface. Figure 2 (a), (b), (c), (d), (e), (f) and (g), shows that potential (V (r), au) increases in the order red < orange < yellow < green < blue. Also, the color code of these maps varies in the interval from deepest red to deepest blue in the compound, where blue represents the strongest attraction and red the strongest repulsion.

Areas of negative V(r) are commonly found in the case of a lone pair of electronegative atoms. From the MEP map of the molecule title, the regions having the negative potential are above the electronegative atom (oxygen atom), and the regions having the positive potential are above the silicon atoms.

Figure 2 (a), (b), (c), (d), (e), (f) and (g), presents the molecular electrostatic potential (MEP) of nanoscale n-fold SiO2 ring clusters at nanoscale n times (n = 2, 3, 4, 5, 6, 7 and 8), respectively. The MEP is a measure of the electrostatic potential at different points around the molecular surface, referring to how a positive test charge would interact with the molecular charge distribution. The MEP is colour-coded by potential values, from red (negative) to blue (positive). The MEP can give information on the stability and polarity of the clusters, as well as the distribution of the electron density and the charge.

The SiO_2 ring clusters consist of a ring of alternating silicon (Si) and oxygen (O) atoms. Silicon atoms are shown in grey, and oxygen atoms are shown in red. The clusters have various planar folds that control their geometries and electrical properties. The planar fold is the number of atoms in the smallest ring that encompasses the cluster. Given that the cluster has a planar fold of 4 since it is in a four-membered ring. In the case of an n=3 cluster, the planar fold is 6 which is present in six-membered rings, and so on.

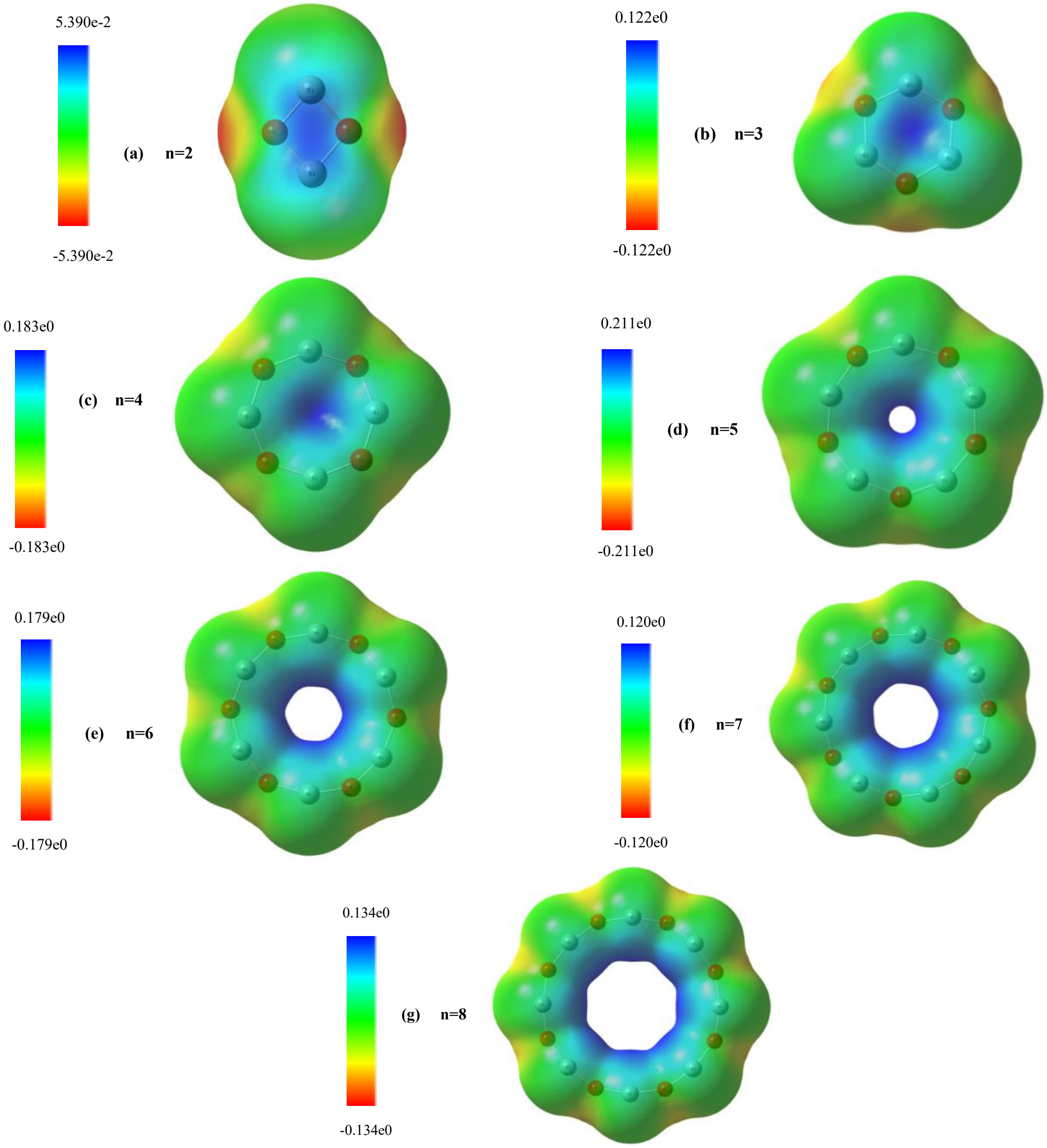


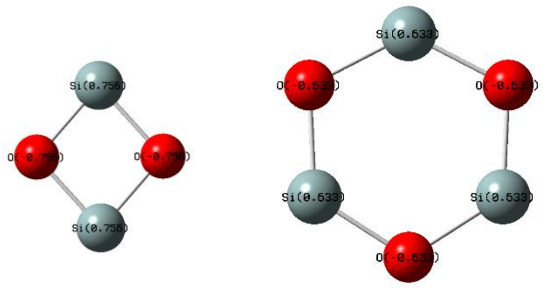
Fig. 2. The figure shows the Molecular electrostatic potential energy maps of the molecular electrostatic potential of the n-fold nanoscale SiO_2 ring clusters, denoted as (a), (b), (c), (d), (e), (f) and (g) for values of n equal to 2, 3, 4, 5, 6, 7, and 8, respectively.

The MEP energy maps show the oxygen atoms as the most negative potential values, denoting them as the most electron-rich and nucleophilic sites in the clusters. The silicon atoms exhibit intermediate potential values, indicating that they are less electron-rich and less nucleophilic compared to the oxygen atoms. Nevertheless, the extent of the above difference is insignificant. The regions between silicon and oxygen atoms carry the maximum positive potentials, which denotes them as the most electrophilic regions of the clusters. In addition, these regions are the most polarized because nearby atoms have low electron density and pull electrons strongly toward them.

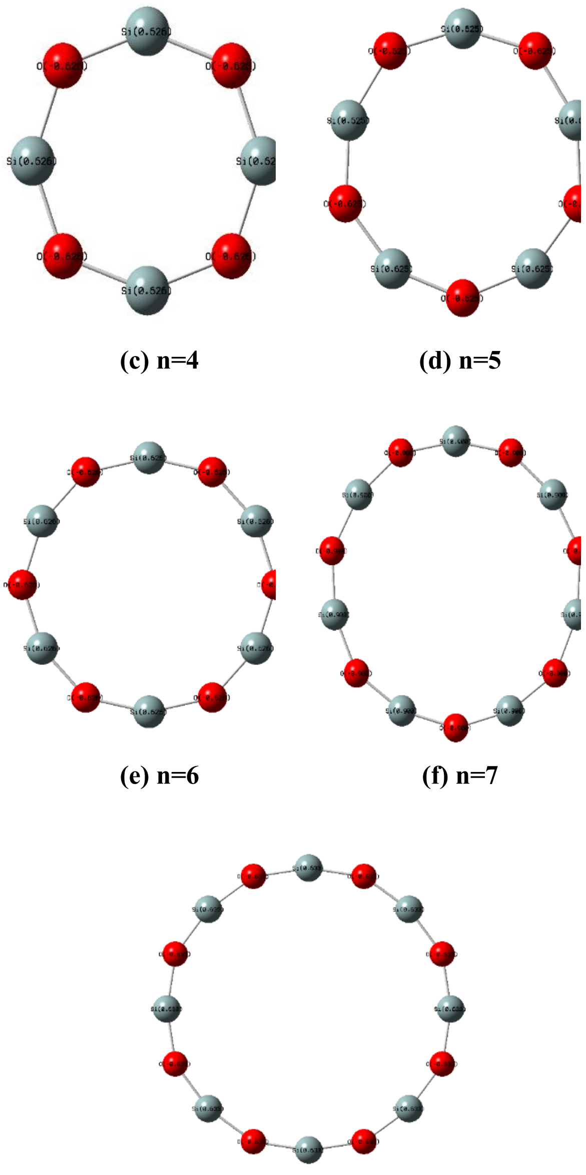
The MEP energy maps further show that the clusters have different electrostatic potential patterns because of their planar folds. The clusters of the coiled nucleus are arranged so that their potential values are equally distributed because the coiled nucleus has numbered circular folds. The lack of symmetry increases the cluster's negative charge and makes it more nucleophilic. Furthermore, the symmetry of the clusters has consequences for the stability of the clusters, as it establishes the sites that are favoured or unfavored for the electrophilic or nucleophilic attack.

In general, Fig. 2(a)–(g) presents the MEP maps of nanoscale n-fold SiO_2 ring clusters, which can be used to study their stability and polarity. The MEP maps reveal that oxygen atoms are the most nucleophilic, silicon atoms are less nucleophilic, and the regions between them exhibit the highest electrophilic character in the clusters. The MEP energy maps also show that clustering upon the planar folds results in different electrostatic potential patterns, thereby influencing the symmetry and stability properties of the clusters.

The study on the stability of nanosized SiO_2 ring clusters is carried out by analysing the Mulliken atomic charges of planar folds with the density functional theory (DFT)method. Models based on Mulliken atomic charges provide information about electron density distribution within the clusters which is essential for interpreting their stability. The Mulliken atomic charges of various planar folds in the SiO_2 ring clusters were obtained using DFT calculations, as shown in Figure 3 By comparing the Mulliken atomic charges across different folding planes, the researchers evaluated the reactivity of the clusters and identified the most stable configurations.



(a) n=2 **(b) n=3**



(c) n=4 **(d) n=5**

(e) n=6 **(f) n=7**

(g) n=8

Fig. 3. The figure shows the Mulliken atomic charge calculation of n-fold SiO_2 ring clusters, indicated as (a), (b), (c), (d), (e), (f) and (g) for values of n equal to 2, 3, 4, 5, 6, 7, and 8, respectively.

Figure 3 (a–g) presents the Mulliken atomic charges of the silica nano finger ring clusters with different planar folds. Mulliken atomic charges are determined by dividing the electron density of each atom into equal parts, corresponding to the number of bonds it forms. They show the electron delocalization within the clusters, affecting their dipole moments, polarizabilities, and reactivities.

The Si atoms (grey) contain positive charges, showing that they have no electrons, thus behaving as very electrophilic sites. The oxygen atoms (red) with negative charges indicate that they are electron-rich, and therefore, they function as the nucleophilic sites. This reflects the difference in electronegativity between silicon and oxygen, with oxygen being more electronegative and thus more electrophilic than silicon. The charges on silicon and oxygen in the plane depend on the planar fold of the cluster. Usually, the larger the planar fold, the lower the charges on the atoms. Such an argument implies that the clusters with larger planar folds are more stable and less reactive than the clusters with smaller planar folds, since they feature lower charge separation and lower electrostatic potential energy.

Depending on the positions and coordination numbers, the charges on the silicon and oxygen atoms in the cluster are different. For example, in the n=4 cluster, the central silicon atom on the ring has a higher positive charge (+0.211) than the corner silicon atoms (+0.183). This is because the central silicon atom has a higher coordination number (four) than the corner silicon atoms (three). Therefore, it shares more electrons with the oxygen atoms and becomes more electron deficient. The positively charged character of central silicon atoms (+0.211) in the n=4 SiO_2 ring cluster exceeds the corner silicon atoms (+0.183) because their coordination number has a significant effect on the electron density distribution. Among Si atoms central positions exhibit the highest number of oxygen bonds, which leads to their extended connection pattern compared to those found at cluster corners. Central Si atoms obtain stronger electron withdrawal from electronegative oxygen atoms around them, thereby accumulating a greater positive charge.

The Lewis acidity of Si atoms increases with greater positive charge because Lewis acids accept electron pairs. The catalytic properties of SiO_2-based materials improve when their Lewis acidity increases specifically in reactions involving electron-rich species [37]. The catalytic properties of the SiO_2 clusters are influenced by the coordination environment of their constituent Si atoms which determines their electron density.

Analogously in the n = 6 group, the oxygen atoms on the edges of the ring have higher negative charges (-0.179) than the oxygen atoms inside the ring (-0.120). This is because there are lower coordination numbers (two for edge oxygen atoms and three for the inner ones) for the edge atoms than the others, which imply higher electron retention and as a result they are more electron rich.

Ring asymmetry in n=7 planar clusters creates non-uniform atomic arrangements between the silicon and oxygen cluster atoms. The irregular ring structure produces an uneven distribution of electrons which results in a non-homogeneous charge distribution. Overall, the electron distribution across the atoms displays an uneven pattern where oxygen atoms hold greater negative charge compared to adjacent silicon atoms which show greater electron deficiency. High electron densities within specific areas transform those regions into active spots that attract nucleophilic reactions.

Localization of reactive sites creates difficulties during catalyst design processes. Having high local reactivity helps speed up specific reactions, but simultaneously triggers instability in the overall system. The unbalanced electronic arrangement makes molecule surfaces more polarised, which potentially leads to deleterious reactions and structural changes throughout use. Developing stable catalytic systems from asymmetric clusters requires scientists to find a precise equilibrium between the activation of reactive sites and the maintenance of structural resilience against degradation under working conditions.

The stability grows in larger planar SiO_2 ring clusters (eg, n = 8) because the symmetry and coordination improve the distribution of charges and decrease the energy of electrostatic potential energy. The Molecular Electrostatic Potential (MEP) maps combined with Mulliken charge analysis show that extended clusters achieve better charge distribution, which prevents localized electrostatic potential concentrations. Internal electrostatic repulsion forces weaken when the system attains uniformity, resulting in reduced potential energy to stabilize the structure. The electronic charge distribution in symmetric structures spreads according to quantum theory, which minimizes electron-electron repulsion to stabilise the structure. DFT investigations have established that symmetric SiO_2 clusters with better coordination patterns result in more stable configurations.

A reduction in charge separation in groups with n values between 6 and 8 generates even electrostatic potential across SiO_2 ring surfaces. The installation of surface uniformity effectively blocks high-potential leak spots that function as current pathways that lead to improved signal quality in OEO systems. Similar findings appear in the report of Wang et al. (2023) when they demonstrated how SiO_2 composite passivation reduced surface leakage currents in InAs/GaSb photodiodes. We believe that the static DFT methods applied in our study validate the findings indicating that enhanced signal integrity results from better passivation because higher-fold clusters exhibit reduced charge separation. The results provide valuable insights on the structural stability of SiO_2 ring nanoclusters of SiO_2 rings and can help develop and implement innovative materials exhibiting the required characteristics.

4. CONCLUSIONS

In this study, several aspects of the stability of nanoscale SiO_2 ring clusters were addressed by applying the DFT method for the calculation of their electrostatic potential energy maps and Mulliken atomic charges. The results emphasise the necessity to know the Coulombic properties of such collections, to create new materials with the needed stability. The MEP energy maps have proved the existence of electrophilic centres on the silicon atoms, and nucleophilic sites on the oxygen atoms inside the oxygen-silicon ring. Thus, they play a significant role in chemical reactions and adsorption mechanisms. Additionally, the rise in the lysosome folds promotes a more uniform distribution of the electrostatic potential and increases the stability but decreases the stability of the clusters. The Mulliken atomic charge measurements reveal that the central silicon atoms experience an increment of positive charges because of tight coordination, while the edge oxygen atoms have more negative charges. The charge transport specific to the positions and sites within the clusters plays a crucial role in the total stability of the clusters. DFT calculations in combination with the electrostatic potential energy maps analysis and Mulliken charges analysis represent a powerful means for the study of the chemistry and stability of silica ring clusters. The results of the presented study can be used as a foundation for designing and creating materials with given properties, especially in catalysis, sensors, and nanotechnology. Comprehensively, this study is a contribution to the growing area of nanoscale systems engineering, where the critical features are the level of understanding of the complex details of charge distribution and the electrostatic properties that determine the stability of nanomaterials. More research can be performed based on the results of this study and additional associated factors influencing the stability mechanisms of SiO_2 ring clusters will be explored in future work. This will expand the applicability of these unique nanomaterials in vast areas.

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Data Availability: Data are available.

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