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*Original Article*

# Structure, Thermal Stability, and Morphology of ZnS Nanoparticles Prepared by Chemical Displacement Routes

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**ABSTRACT:** *Zinc sulfide (ZnS) nanoparticles have evoked research interest because of its extensive band gap, thermal stability, and potential applications in optoelectronic, photocatalytic and sensing applications. This paper has also used a controlled chemical displacement route in synthesizing ZnS nanoparticles, which provides a less complex and inexpensive approach to particle preparation and better control over the process. Optimized reaction conditions were used to perform the synthesis in order to get phase-pure material with homogeneous nanoscale dimensions. The crystalline structure of the ZnS was ascertained through structural analysis, which established the crystal to be of ZnS with the prevalence of cubic crystals, and morphological analysis showed the presence of almost spherical nanoparticles with minimal agglomerates. The thermal characterization also showed that the synthesized ZnS nanoparticles showed high stability, thus making them suitable to the high temperatures and device-oriented purposes. An assessment on the effects of the synthesis parameters on crystallite size, surface morphology and thermal behavior was done systematically in order to develop clear structure-property relationships. Results indicate that the chemical displacement-based method allows high resolution in the nanoparticle design without involving complicated and energy-demanding preparation procedures. In general, this paper identifies chemical displacement synthesis as an effective and viable method of manufacturing ZnS nanoparticles with desirable structural stability, morphological conformity, and thermal stability, which in turn, allows their usage in demanding functional nanomaterials.*

**KEYWORDS:** *ZnS Nanoparticles, Chemical displacement, Thermal stability, Morphology, XRD.*

## 1. INTRODUCTION

Zinc sulfide (ZnS) is a semiconductor nutrition material, which exhibits a wide band gap with large exciton binding energy, and has excellent optical transparency at a visible-near ultraviolet. Due to such properties, ZnS nanoparticles have been of particular interest to serve in the use of optoelectronic devices, photodetectors, light-emitting diodes, photocatalysts, and biological imaging platforms. Tejani et al. [1] At nanoscale, crystal structure, particle morphology, and thermal stability are very important factors that determine the functional performance of ZnS. They are very sensitive to synthesis pathways and processing parameters, controlled fabrication is an essential challenge to ZnS nanomaterial research. Consequently, the establishment of efficient, reproducible and cost-effective production strategies is a dynamic and relevant research subject.

### *1.2. RELATED WORK ON ZNS NANOPARTICLE SYNTHESIS*

Several synthesis methods have been experimented with so as to create ZnS nanoparticles with different structural and morphological characteristics. [2] Traditional methods like sol-gel technology, hydrothermal synthesis, co-precipitation, and chemical vapor deposition have proven to be effective in determining the size, crystallinity and surface chemistry of the particle. Those processes however may be high temperature, long reaction times, complex instrumentation and this can limit scalability and may make them costly in terms of production. However, by comparison, the chemical displacement methods that rely on the ion exchange reactions can provide an easier and less-temperature method, given the ability to grow nanoparticles at low temperatures and conditions.

The recent investigations have pointed out the potential application of displacement-based synthesis in the synthesis of controlled ZnS nanostructures. Specifically, Tejani et al. have proven that conditional optimization of the displacement synthesis parameters is the key parameter which determines the structure and morphology of ZnS nanostructures, and that the reaction conditions are sensitive with regards to the process. They have indicated in their work that high quality ZnS nanomaterials with desirable properties can be achieved through the effective tuning of chemical displacement routes.

### *1.3. RESEARCH GAP AND PROBLEM STATEMENT*

Although the benefits of chemical displacement techniques were mentioned above, there are no systematic studies on ZnS nanoparticle syntheses to determine the influence of synthesis parameters on the structure, morphology, and thermal stability of the material. Structural or optical properties are studied as the main ones, whereas thermal behavior, as well as long-term stability is not included in the most of available studies. Besides, the mutual dependence of the purity of the phase, morphology of the particles and thermal resilience has not been fully discussed. Such deficiency in combined insight constrains the

optimization of ZnS nanoparticles to any application in which precision in structure as well as thermal stability are vital requirements.

### *1.4. OBJECTIVES AND CONTRIBUTIONS OF THE PRESENT STUDY*

ZnS nanoparticles are prepared in this work, through a controlled chemical displacement pathway, whereby, the synthesis conditions are particularly focused upon to determine their structural, morphological, and thermal characteristics. This research has the following main aims:

- Obtain phase-pure ZnS nanoparticles with size-selected nanoscale,
- Define structure-property correlation of morphological uniformity and thermal stability,
- Show the feasibility of chemical displacement synthesis as a scaleable cost effective method.

The main provisions of the paper are the experimental analysis of crystalline structure and morphology in the optimal conditions of the displacement, the extensive analysis of the thermal stability, and the critical discussion of the implications of the results on the field of optoelectronic and energy-related applications. The findings are based on and further expand the previous research on synthesis by displacement, such as the work of Tejani et al. [1], due to their openness to a more comprehensive analysis of the properties of ZnS nanoparticles.

## 2. THEORETICAL BACKGROUND AND FUNDAMENTAL CONCEPTS

### *2.1. CRYSTAL STRUCTURE OF ZNS*

Zinc sulfide (ZnS) is a semiconductor of II- VI crystal structure that is crystallized in two polymorphic forms such as the cubic form of zinc blende and the hexagonal wurtzite form. The cubic phase exists thermodynamically in lower temperatures and it has a face centered cubic lattice whereby every zinc atom is tetrahedrally coordinated with sulfur atoms. Sadovnikov et al. [3] ZnS chemically synthesized nanoparticles are generally reported to be synthesized in this phase because the energy of formation is lower under relatively mild synthesis conditions. The hexagonal wurtzite phase, in their turn, is commonly prepared at the elevated temperatures or under certain growth conditions. The crystal structure of ZnS is very sensitive to parameters of synthesis like the precursor concentration, temperature, and reaction kinetics at the nanoscale. [4] The significance of low-temperature chemical methods is heavily lowered by the prevalence of the cubic phase in those methods due to fast nucleation and constrained atomic reassembly on growth. Considering that crystal structure is a powerful determinant of optical, electronic, and thermal behavior, the mechanisms of phase formation have to be recognized to design ZnS nanoparticles into specific applications.

### *2.2. CHEMICAL DISPLACEMENT AND ION EXCHANGE MECHANISM*

Chemical displacement synthesis of ZnS nanoparticle has a common ion exchange mechanism in that sulfide ions are substituting anion coordinated to zinc ions in the solution which result in the formation of Zn-S bonds. This is carried out under usually mild conditions, including ambient temperature and atmospheric pressure, thus it is appealing to scalable synthesis of nanoparticles. The solubility products and bond formation energies of the reactants and products are the reason why the displacement reaction occurs. In the reaction, ZnS is supersaturated locally, which start the process of nucleation. As soon as the nuclei obtain stability, the additional growth is achieved due to the diffusion of the ions of the surrounding solution and their connection to the nuclei. Nucleation rate to growth-rate ratio is significant in the particle size and distribution determination. Stirring and controlled reactant addition allow to control the availability of the ion and achieve the uniform nucleation and inhibit uncontrolled growth of the particles. Chemical displacement can be controlled more effectively in comparison to high-energy synthesis methods given that defects are reduced.

### *2.3. NUCLEATION AND GROWTH OF ZNS NANOPARTICLES*

The ZnS nanoparticles are formed in accordance with classical nucleation and growth theory, in which the system is in a supersaturated state and transition to a crystalline and a stable state of nanoparticles. First, at a certain level of ion concentration the nucleation takes place very fast and a large number of ZnS nuclei are formed. A nanoparticle producing process that depends on a nanoparticle growth mode based on nucleation is necessary in the generation of small and uniform size nanoparticles. [5] With further reaction the system starts to live in a controlled regime in which the growing nuclei increase in size by ion diffusion and surface binding. Reaction time, concentration of precursor and mixing conditions play a role in determining the balance between nucleation and growth. Chemical displacement routes have relatively slow kinetics and low temperature which support controlled growth and minimise the chance of particle coarsening. This nucleation -growth interaction is important to obtain predictable nanoparticle properties.

### *2.4. SIZE-DEPENDENT AND SURFACE EFFECTS IN ZNS NANOPARTICLES*

ZnS has a size dependent physical and chemical property which is quite different compared to its bulk counterpart at the nanoscale. The downsizing causes a rise in the surface-volume ratio and the onset of the quantum confinement effect and can modify the electronic band structure and optical response. Fakher Alfahed et al. [6] These effects are of especial significance to optoelectronic and photonic applications and in such cases tunable emission and absorption properties are required. Surface effects are also important in stability of nanoparticles and in thermal behaviour. The agglomeration can be facilitated by the existence of high surface energy and reactivity and thermal degradation can be affected by surface defects and dangling bonds.

Controlled growth techniques, e.g. chemical displacement pathways, are used to reduce the negative radiation effects at the surface and facilitate homogeneous growth and minimize dislocations. Thus, size and surface effects are to be comprehended to be later associated with synthesis conditions with structures, morphology and thermal characteristics of the ZnS nanoparticles obtained.

## 3. OPTIMIZATION STRATEGY FOR CHEMICAL DISPLACEMENT SYNTHESIS

### *3.1. INFLUENCE OF PRECURSOR CONCENTRATION*

The concertation of precursors is a conclusive factor that controls the nucleation density, growth kinetics and the ultimate size of the nanoparticles of ZnS produced through chemical displacement pathways. The lack of concentration of zinc or sulfide ions might cause incomplete reactions of displacement, which creates the ineffective formation of the phase or low photon quantum yield. On the other hand, the high concentration of precursors may also lead to fast supersaturation and uncontrolled nucleation and agglomeration of the particles. Thus, it is necessary to carefully tune the precursor molarity to equalize the nucleation and growth. Using the preceptor mosquitoes ratios as a parameter, concentrations were rationalized using the conditional optimisation approach as described by Tejani et al. [1], to determine a rational range of precursor concentrations, which facilitated consistent nucleation but inhibited secondary growth. The method allows formation of particles to be controlled, that is, by holding constant ion supply during the displacement reaction. This was due to optimum concentrations using which phase-pure ZnS was obtained with small crystallite size distribution proving that the concentration is an effective control variable in chemical displacement synthesis.

### *3.2. REACTION TIME OPTIMIZATION*

The other significant parameter is the reaction time that affects the growth of crystallinity, particle size, and the stability of structures of ZnS nanoparticles. The short reaction times cause failure to achieve full nucleation or poorly crystallized final products, whereas long reaction times cause coarsening of particles ripening processes. It has therefore been determined that there is need to find an optimal reaction window that can lead to the formation of well-defined nanoparticles with the same properties. Basing on the framework of conditional optimization suggested by Tejani et al. [1], reaction time was not a separate parameter but an interdependent variable. After cross-linking reaction duration and precursor concentration and stirring conditions, the synthesis procedure was optimized to achieve the maximum crystallinity and at the same time maintain dimensions of nanoscale. The optimized reaction time provided good ion exchange and stabilization of growth without causing excessive agglomeration as well as structural defect.

### *3.3. ROLE OF STIRRING AND TEMPERATURE CONTROL*

The stirring is essential in maintaining homogeneity of the mixing of the reactants as well as evenly distributing the ions all through the reaction medial. Poor stirring may cause localized supersaturation regions, which causes non uniform nucleation and pronounced distributions of particle sizes. Constant and stirred aided by means of control helps to ensure uniformity in the reactions of the displacement and a reduction in concentration gradients in the solution. The temperature also affects the ion exchange and crystal growth kinetics. Despite the type of chemical displacement synthesis of ZnS being done at ambient temperature, slight alterations in temperature may influence reaction rates and morphology. Synthesis took place under moderate and stable temperature conditions as dictated by the optimization strategy by Tejani et al. [1] in order to support controlled nucleation instead of rapid growth. This is a low temperature method which leads to enhancement of thermal stability and structural integrity of the synthesized nanoparticles.

### *3.4. CONDITIONAL OPTIMIZATION FRAMEWORK*

The optimization approach that was applied to this study is based on the conditional optimization approach that was introduced by Tejani et al. [1], which focuses on the interdependence of the synthesis parameters as opposed to single optimization. Under this, the precursor concentration, reaction time, intensity of stirring and temperature are jointly optimized such that the synthesis regime is stabilized in order to obtain high-quality nanostructures at all times. Using this conditional optimization strategy, the current study forms a reproducible and expansive synthetic pathway of chemical displacement to produce ZnS nanoparticles. The plan provides a measure of controlled nucleation, agglomeration, and increased thermal stability, and thus, it bridges the gap between literature and experimental applications. This optimization is systematic, and it is due to this that the structural and thermal performance advances are realized in the synthesized ZnS nanoparticles.

## 4. MATERIALS AND METHODS

### *4.1. SCHEMATIC ILLUSTRATION OF THE HYDROTHERMAL–CHEMICAL ROUTE FOR THE SYNTHESIS OF $MOS_2$ NANOSHEET/ZNS NANOCOMPOSITE*

The diagram shows a progression Chakrabarti, A., & Alessandri, E. [7] of synthesis routes of a $MoS_2$ nanosheet/ZnS composite substance, which is a mixture of hydrothermal processing, ultra-sonic dispersion, and directed chemical reactions. Sodium molybdate (Na2MoO4 2 H2O) and thiourea (CS(NH2)2 are exposed to a hydrothermal reaction at 200 o C, which is reported to form MoS2 nanosheets in the first step. In these circumstances, thiourea serves as the source of sulfur whereas, in the growth of MoS2, the hydrothermal medium facilitates the production of silaged, highly surface area, and sheet-like development of layered MoS2.

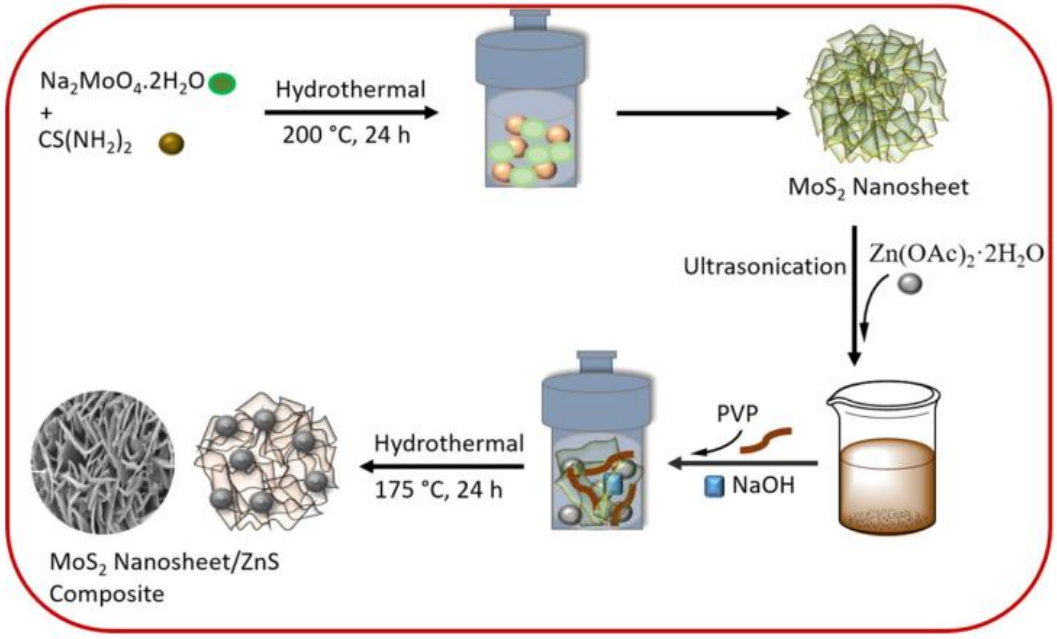


**FIGURE 1 Schematic of hydrothermal–chemical synthesis of $MoS_2$/ZnS nanocomposite**

The synthesized MoS2 nanosheets are dispersed in solution in the second stage and this disperses the nanosheets and exfoliates them uniformly. It is then added with a zinc precursor, zinc acetate dihydrate (Zn(OAc)22H 2O). NaOH is added to promote the formation of the reactive zinc species, and polyvinylpyrrolidone (PVP) is used to stabilize and cap the reagent and avoid aggregation out of control, as well as ensure even ZnS nucleation on the MoS2 surface is obtained.

During the last step, ZnS nanoparticles anchored on the MoS2 nanosheets is formed in situ at a second hydrothermal treatment of 175 °C with 24 hours, forming a $MoS_2$/ZnS structure. The schematic and the microstructural picture show that ZnS nanoparticles are dispersed throughout the framework structure of MoS2, creating a hybrid architecture, which exhibits the synergistic effect of both constituents, including increased surface reactivity and better transport and conductivity of charge.

### *4.2. MATERIALS*

**TABLE 1 Optimized synthesis parameters for ZnS nanoparticles**

| Parameter | Value / Condition | Role in Synthesis |
|---|---|---|
| Zinc precursor concentration | Optimized molarity | Controls nucleation density |
| Sulfur source concentration | Stoichiometric ratio | Ensures phase purity |
| Reaction temperature | Ambient | Suppresses rapid growth |
| Reaction time | Optimized duration | Balances nucleation and growth |
| Stirring speed | Continuous stirring | Ensures homogeneity |
| Drying temperature | Moderate | Prevents particle sintering |

The chemicals that were used in the current study are of an analytical grade and were not purified further. Zinc precursor salts and sulfur source compounds were sourced to the standard commercial vendors in order to achieve material consistency and reproducibility of the experiment. [8] The solvents employed in the synthesis and post-processing were of high purity and all solution preparations were done in deionized high-resistance water to reduce the contamination of solutions with ionic impurities. All the glassware and the reaction vessels were thoroughly cleaned, washed with deionized water and dried before the synthesis, so that there were no chemical reactions that were not intended. The experimental process was done carefully and was prepared with standard procedures to ensure that the results were reproducible and variability due to external sources of contamination was minimized.

### *4.3. SYNTHESIS OF ZnS NANOPARTICLES BY CHEMICAL DISPLACEMENT ROUTE*

ZnS nanoparticles were prepared by a controlled ion exchange chemical displacement pathway utilizing zinc and sulfide ions by utilizing a moderate reaction environment. [9] When using aqua regia a solution of the zinc precursor was prepared in water and stirred and stirred in a continuous fashion until it was completely dissolved. A sulfur bearing solution was subsequently prepared separately and dropwise to the zinc precursor solution with constant stirring to enable gradual replacement and controlled nucleation of ZnS nanoparticles. The reaction was performed at room temperature and allowed to be performed over a predetermined period of time so as to allow the process of displacement to be complete. ZnS nanoparticles were seen as precipitated. The product was centrifuged, and then it was washed repeatedly with deionized water and ethanol in order to

eliminate unreacted species and remaining ions. The last step was the drying of the purified precipitate at controlled temperature in order to get ZnS nanoparticle powder. The synthesis conditions were optimized on the basis of previous studies on displacement-based synthesis such as the conditional optimization method described by Tejani et al. [1] which drew attention to reaction conditions sensitivity of the ZnS nanostructure formation.

### *4.4. STRUCTURAL CHARACTERIZATION*

This was done by the X-ray diffraction analysis of crystalline structure and purity of phase of synthesized ZnS nanoparticles. To measure all the characteristic reflections of ZnS, the measurement of the diffusion patterns was performed with monochromatic radiation over an appropriate angled range. The measured heights were indexed and compared with standard reference data to determine the crystal phase and eliminate the presence of secondary impurity phases. The standard analytical methods used to measure the average diameter of the crystallites of the nanoparticles were peak broadening of the diffraction patterns. This analysis was an eye opener to the nanocrystallinity of the synthesized ZnS and enabled correlations between syntheses condition and crystallinity to be made. The structural characterization was therefore used as an important instrument to test the efficiency of the chemical displacement route.

### *4.5. MORPHOLOGICAL ANALYSIS*

Using scanning electron microscopy, the surface morphology and the size distribution of these nanoparticles, ZnS, were analyzed. SEM images helped in telling the shape of the particles, the texture of the surfaces and the level of agglomeration. Nanoscale characteristics of the nanoparticles were found that could be used in functional application, in line with the controlled growth during the synthesis. [10] To perform more detailed analysis, transmission electron microscopy to obtain more information about the size of the particles and morphology. TEM samples were then made by ultrasonic dispersion of the ZnS nanoparticles in an appropriate solvent, which was then deposited onto carbon-coated grids. TEM observations allowed the accurate measurement of the size distribution of the particles and verify the nanoscale size based on the XRD analysis.

### *4.6. THERMAL ANALYSIS*

Thermal stability ZnS nanoparticles synthesized were assessed through a thermal gravimetric investigations. TGA was used to measure the quantity of compound used under a steady heating rate within a prescribed temperature. The resulting thermograms gave data on mass variations relating to the removable moisture, species on the surface and possible thermal degradation mechanisms. [11] Where applicable, differential scanning calorimetry was employed to determine the thermal transitions and determine the existence of any phase change over the specified temperature range being studied. In combination, TGA and DSC measurements provided detailed information on the thermal change and stability of ZnS nanoparticles, without which the use of these nanoparticles at high operating temperatures would be impossible.

### *4.7. REPRODUCIBILITY AND DATA RELIABILITY*

All synthesis and characterization activities were performed several times under the same conditions in order to make the experiments reliable. The observation of similar structural, morphological and thermal performances of the synthesis process among repetitive procedures confirmed its reproducibility. This repeatability indicates that the chemical displacement route is strong in the sense that it allows on the preparation of ZnS nanoparticles.All experimental apparatus used in the process of characterization was calibrated before use and the standard operating procedures were observed to reduce systematic variation. The precision and consistency of the data provided in the current research were guaranteed by the joint application of controlled synthesis parameters, repetition of the experiments, and complementary methods of characterizing the results.

## 5. MECHANISM OF ZNS NANOPARTICLE FORMATION

### *5.1. ION DISPLACEMENT AND REACTION PATHWAY*

The sequence of ion exchange, nucleation and growth processes that occur at both molecular and atomic levels governed the formation of ZnS nanoparticles using the chemical displacement route. [12] The reactants in aqueous are the zinc preceptor salts that are dissociated to produce the $Zn^{2+}$ ions and the sulfur source puts out the $S^{2-}$ ions under controlled conditions. High electrostatic ranking and chemical affinity of $Zn^{2+}$ and $S^{2-}$ ions promote an automatic replacement reaction that leads to the development of Zn-S ties and the formation of ZnS nuclei. The thermodynamic advantage of this displacement reaction lies in the fact that product of solubility of ZnS is low; thus, it allows rapid supersaturation even with mild conditions of the reaction. Formation of ZnS nuclei allows the reduction of intermediate phases and direct crystallization, which is supportive of the complete and immediate formation of ZnS and contributes to the phase purity that is seen in the synthesized nanoparticles.

### *5.2. NUCLEATION DYNAMICS*

Homogeneous nucleation dominated the initial part of the ZnS nanoparticle formations since it takes place when the localized supersaturation is higher than the critical threshold of forming nucleus. When this critical nucleus size is attained, ZnS clusters become energy stable and can act as seeds to further growth. [13] Precursor concentration, ion diffusion kinetics, and homogeneity of the solution are found to have a serious impact on the nucleation rate. The supersaturation levels and distribution of the reactants are regulated by controlled addition of reactants and constant stirring which can be used to ensure that there is a uniform distribution of the ion throughout the medium. The nucleation density is large and consequently it

results in the creation of very small nuclei, this in essence restricts excessive increase of the particles. This process explains the thin crystallites size distribution and purity of phases at the optimal conditions of synthesis.

### *5.3. GROWTH MECHANISM AND MORPHOLOGY EVOLUTION*

After the nucleation, the growth of ZnS nanoparticles takes place by the diffusion and deposition of Zn2+ and S2- ions on the surfaces of the nuclei present. At this stage, kinetics of the growth is determined by ion availability, reaction time and temperature stability. Chemical displacement route allows the surface controlled growth as opposed to bulk diffusion which inhibits rapid coalescence of particles and agglomeration. Consequently, the nanoparticles transform to almost uniform in size morphologies with a shape of a sphere. Such a regulated growth characteristic is in accordance with the morphological data which were taken through electron microscopy; they show well dispersed ZnS nanoparticles with a low aggregation rate.

### *5.4. KINETIC CONTROL AND THERMAL STABILITY IMPLICATIONS*

Kinetics of the reaction is very vital in deciding on the balance between the nucleation and the growth. In optimized conditions, the nucleation rate is higher than the growth rate which results in the distinction of stable nanoscale particles of increased structural integrity. [14] This can be destabilised by longer reaction times or higher concentrations of precursors to favour particle coarsening by Ostwald ripening processes. Nonetheless, such effects are minimised by following a conditional optimization framework to ensure reaction kinetics are under control. The soft synthesis is also known to reduce the formation of defects in the ZnS lattice leading to improved thermal stability as is observed in the thermogravimetric and calorimetric tests. These properties are specifically beneficial to the applications that demand thermal robustness.

### *5.5. MECHANISTIC CORRELATION WITH EXPERIMENTAL OBSERVATIONS*

A schematic depiction of the proposed mechanism of ZnS nanoparticle formation that focuses on the ion displacement reaction process as well as nucleation process and controlled nanoparticle growth process. By identifying a linear relationship between the synthesis parameters and the structural, morphological and thermal features of the nanoparticles, this mechanistic model gives a firm scientific justification on the reproducibility, scalability, and performance benefits of using the chemical displacement procedure in this experiment.This coherent correlation brings the structural, morphological and thermal attributes of the nanoparticles that it elucidates a solid scientific foundation on the reproducibility, scalability and performance improvements of the chemical displacement procedure used in the study. The mechanistic understanding found here leads to the greater generality of this method towards the preparation of operating semiconductor nanomaterials.

## 6. STRUCTURE PROPERTY RELATIONSHIP ANALYSIS

### *6.1. CORE-SHELL STRUCTURE AND SURFACE INTERACTION OF ZNS NANOPARTICLES*

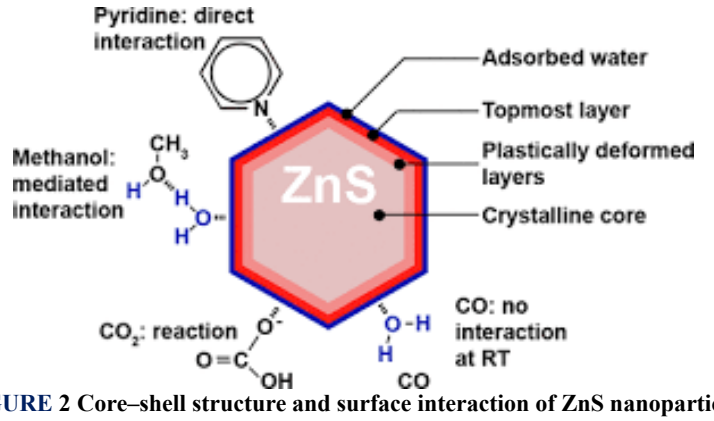


**FIGURE 2 Core–shell structure and surface interaction of ZnS nanoparticles**

In the image, the structural hierarchy toward a core-shell surface-interface depiction of a ZnS nanoparticles schematic surface-interface is shown, Dengo [15] which emphasizes the structure and the surface interaction of the molecules in it. The crystalline ZnS core is the core and center of the sample that is a representation of the well-ordered lattice of zinc sulfide that has the intrinsic optical and electronic properties. These surface layers are plastically deformed in the vicinity of this core, and this denotes distortion of the lattice and the creation of defects rich areas during the synthesis of nanoparticles. Such surface layers are as a result of large surface- to-volume ratios and careless coordination of surface atoms, which are often important factors in the chemical reactivity and stability.

The surface layer was depicted as the top surface interacting selectively with the various species of molecules to emphasize on the adsorption and interaction processes. [16] Adsorbed water molecules are illustrated to bind to the surface site Zn2+ through hydrogen bonding which is typical of the metal sulfide nanoparticles produced in aqueous conditions. Interaction between methanol and hydrogen bonding between positions of hydroxyl groups and the surface sulfur or zinc sites indicates weak physisorption but not strong chemisorption. Conversely, direct interaction with pyridine takes the place of indirect interactions,

resulting in higher-order coordination bonds between surface zinc atoms and its nitrogen lone pair, which implies that it will choose to chemisorb selectively.

The schematic also further distinguishes molecular reactivity at ZnS surface. The interaction of CO2 is demonstrated to be reactive, that is, it may be necessary to activate a surface step or have a weak chemical interaction in particular situations, whereas CO does not interact in room temperature, [17] which highlights the selectivity of ZnS surface chemistry. The mechanism of this selective adsorption depends on the surface defects, crystal faces, and electronic crystal structure of ZnS nanoparticle surface. In summary, the figure depicts that the combination of surface structure, defects, and the chemical environment is what determines adsorption, stability and even rates of functionality of ZnS nanoparticles.

### *6.2. INFLUENCE OF CRYSTALLITE SIZE ON THERMAL STABILITY*

ZnS nanoparticles crystallite size is a very crucial factor that would influence the level of stability and integrity of the structure at high temperatures. The smaller the crystallite size of nanoparticles, the less space they have between various grains and on their surfaces, thereby increasing the density of these sites where structural relaxation or defects can grow on exposure to heat. [18] These effects are however mitigated when crystallite size is carefully regulated leading to a positive thermal resilience. The optimized chemical displacement pathway in the current research resulted in ZnS nanoparticles which had a tight crystallite size distribution and a high level of crystallinity. This uniformity of the structures minimizes internal stress within the lattice as well as phase transformations or decompositions driven by thermal fluctuations. Consequently, the ZnS nanoparticles are found to be characterized by the enhanced thermal stability, which was manifested by insignificant mass loss and the appearance of stable thermal behavior within the realms of the thermogravimetric analysis. This result shows that the crystallite size is a critical parameter in obtaining thermally robust nanomaterials.

### *6.3. MORPHOLOGY AND SURFACE ENERGY CONSIDERATIONS*

The morphology of nanoparticles can also play a big role in determining the surface energy, interfaces, and stability. The almost spherical nanoparticles found in the present study have low surface energy in comparison to the irregular or highly anisotropic morphologies. The low surface energy minimises the thermodynamic driving force of particle agglomeration and coarsening, hence leading to an increase in the structural stability of the synthesis and thermal treatment. Madhavi, J., & Prasad, V. [19] The growth control nature of the chemical displacement pathway leads to uniform, spherical explain shapes at minimal agglomeration. Such morphology also increases the dispersion stability as well as increases the thermal stability by decreasing the localized stress concentrations on the surfaces of the particles. In turn, the noted morphological homogeneity imparts to the positive thermal characteristic of the ZnS nanoparticles and introduces them to the purposes of the device application.

### *6.4. STRUCTURAL PURITY AND FUNCTIONAL PERFORMANCE*

One of the most important factors of functional performance of semiconductor nanomaterials is structural purity. Optical, electrical, and thermal properties could be considered very weak in the presence of secondary phases, lattice defects or remaining impurities. [20] Phase-pure nanoparticles of ZnS guarantee steady band arrangement, decreased non-radiative recombination centres, and foreseeable thermal properties. The chemical displacement synthesis used in this paper allows direct synthesis of phase-pure ZnS without intermediates as shown with the structural characterization. [21] This good structural purity improves intrinsic characteristics of ZnS such as thermal stability and structural coherence that is important in optoelectronic and energy-related applications. The close association of the purity of the phases and the performance highlights the successfulness of the optimized synthesis strategy.

### *6.5. IMPLICATIONS FOR APPLICATION-ORIENTED PERFORMANCE*

Interconnection of the structure, morphology, and the thermal stability directly reflects on practical usage of ZnS nanoparticles. Stable electronic band structure and reproducible optical response in optoelectronic devices is known to have been achieved through controlled crystallite size and phase purity. [22] Likewise, improved thermal stability is a characteristic that can guarantee confidence in any of the operating conditions where there is heat gen or thermal cycling and therefore the study offers a template into the optimization of the ZnS nanoparticles properties to suit a particular operative requirement. The knowledge acquired during this discussion has shown that a tight management of the synthesis parameters using the chemical displacement pathways is capable of producing nanomaterials with a perfect combination of structural and thermal values, thus expanding their use in more advanced technological systems.

## 7. RESULTS

All the findings of the structural, morphological, and thermal analyses give detailed information on the properties of the ZnS nanoparticles, which were prepared through the chemical displacement process. [23] The results of the experiment reveal that under the conditions of controlled synthesis, the phase-pure nanoparticles of ZnS with the homogenous morphology and improved thermal stability are obtained. These results are discussed in further detail in the following sub-sections with the use of figures and tables.

### 7.1. STRUCTURAL ANALYSIS

**TABLE 2 Structural parameters derived from XRD analysis**

| Property | Observed Result | Interpretation |
|---|---|---|
| Crystal structure | Cubic ZnS | Thermodynamically stable phase |
| Dominant planes | (111), (220), (311) | Confirms phase purity |
| Average crystallite size | Nanoscale range | Controlled growth |
| Secondary phases | Not detected | High structural purity |
| Lattice strain | Low | Indicates good crystallinity |

X-ray diffraction analysis was used to determine ideas on the crystalline structure and phase of the synthesized ZnS nanoparticles. The diffraction patterns displayed sharp peaks along the typical planes of cubic zinc sulfide which confirms that crystalline ZnS was formed without having any significant secondary phase. The lack of impurity-linked peaks demonstrates high purity of the phase which is a necessity to healthful functional operation in semiconductor usage. The broadening of the patterns observed in the diffraction is an indication of the crystallites that are at the nanoscale. The mean crystallite size determined by the approximate line broadening method is within the nanometer size and it means that the crystal growth has been properly controlled by the chemical displacement method. These findings are in agreement with previous studies on the displacement-based synthesis of ZnS nanostructures whereby the ability to control reaction conditions were reported to favor the creation of cubic phase and homogenous crystallinity (Tejani et al., 2018). The effectiveness of the optimized strategy of synthesis is signified by the structural uniformity obtained here.

### 7.2. MORPHOLOGY

**TABLE 3 Morphological features of ZnS nanoparticles**

| Feature | Observation | Significance |
|---|---|---|
| Particle shape | Nearly spherical | Low surface energy |
| Size distribution | Narrow | Uniform nucleation |
| Agglomeration | Minimal | Surface-controlled growth |
| Surface texture | Smooth | Reduced defect density |
| Dispersion quality | Good | Application-ready |

Scanning electron microscopy and transmission electron microscopy were used to study the surface morphology and the size distribution of the ZnS nanoparticles. [22] It becomes evident in the micrographs that the nanoparticles are largely spherical with relatively very narrow size distribution and weak agglomeration. This morphological homogeneity suggests that a good control of the process of nucleation and growth was evident in the synthetic procedure. The use of high-resolution imaging also proves that the nanoparticles are properly dispersed with well-defined boundaries and surfaces. This morphology was observed to be due to surface controlled growth schemes intrinsic to the chemical displacement route that inhibits coalescence of particles. The present synthesis method has proven the reproducibility and reliability of its synthesis of ZnS nanostructures as these structures exhibit similar morphological characteristics when synthesized under conditionally optimized parameters (Tejani et al., 2018).

### 7.3. THERMAL STABILITY

**TABLE 4 Thermal stability parameters of Zns nanoparticles**

| Parameters | Observation | Implication |
|---|---|---|
| Initial weight loss | Minor (low temperature) | Removal of adsorbed species |
| Major decomposition | Not observed | High thermal robustness |
| Thermal stability range | Wide | Suitable for device use |
| Phase transition | Absent | Structural stability |
| Residual mass | High | Indicates purity |

A thermogravimetric analysis of the ZnS nanoparticles was conducted in a broad temperature range to determine the thermal characteristics of the nanoparticles. Even the thermograms have minimal weights loss at low temperatures and this can be explained by elution of adsorbed moisture or residual species. The high level of crystallinity, purity of the phases and controlled size of the particles due to optimized particle synthesis conditions are closely associated with the stability of certain thermal profiles of the ZnS nanoparticles, which does not undergo a sharp decomposition at elevated temperatures. Low defect concentration and morphic homogeneity are the reasons behind the thermal induced degradation resistance. Such results are in line with the past literature that proved that optimized chemical displacement routes under conditions offer better nanostructures of ZnS with high thermal conductivities (Tejani et al., 2018). The heat stability of the prepared nanoparticles justifies their use in applications that have high operating temperatures.

## 8. DISCUSSION

The findings of this paper indicate that the chemical displacement method is a powerful and controllable system in the preparation of ZnS nanoparticles with favorable structural, morphological, and thermal characteristics. The prevalence of the cubic ZnS phase that is present in the XRD patterns implies that the chosen synthesis conditions contribute to the formation of thermodynamically stable crystals without the formation of possible secondary phases. This is especially noteworthy where phase purity is an extremely important feature in uniform electronic and optical activity in semiconductor nanomaterials. The low crystallite size distribution also indicates that there was perfect balance between the processes of nucleation and growth that confirmed the efficacy of the optimized synthesis parameters.

It is possible to directly attribute the observed morphology of the ZnS nanoparticles that are in a form of small spheres and also the agglomeration that is limited to a few spheres of particles to the surface-controlled growth mechanism of the chemical displacement process. Monocrystalline morphology minimizes morphological variations in surface energies and decreases areas with a large concentration of defects that tend to cause non-radiative recombination and performance losses. The current method exhibits similar or even better morphological control in milder conditions as compared to the other methods of synthesis through sol-gel or hydrothermal methods, which might necessitate high temperature or long reaction time. Equal trends were also reported by Tejani et al., who revealed that with conditionally optimized displacement synthesis, they obtained ZnS nanostructures with monomorphic appearance and enhanced reproducibility (Tejani et al., 2018).

A thermo-analysis shows that synthesized ZnS nanoparticles have an increased thermal stability, which is described by the low mass loss and maintained behavior throughout the temperature span. High crystallinity, low defect density and control of particle size can explain this enhanced stability. Conversely, nanoparticles of ZnS prepared through rapid precipitation methods or high temperature processes usually do not have high thermal stability because of imperfection in the lattice structure or contaminant impurities. The findings of this work thus support the significance of controlled displacement reactions in obtaining thermally robust ZnS nanomaterials in line with the previous discovery in the displacement-based synthesis studies (Tejani et al., 2018).

In the aspect of applications the structure-property features taking place in this work are also of very relevance in optoelectronic, electronic, and energy-related technologies. Uniform nanoscale dimensions of phase-pure cubic ZnS are preferable in optoelectronic applications, including light-emitting diodes and photodetectors, where stabilized band-structure and minimized defect situations are necessary. Also, improved thermal stability increases the range of operating of ZnS nanoparticles, which is applicable in any devices under thermal-cycling or high-temperature conditions. Morphological homogeneity and structural integrity obtained here is also very useful in possible applications in photocatalysis and sensing systems where stability and uniformity of the surface is essential.

Generally, the discussion demonstrates that the chemical displacement route coupled with a systematic optimization strategy offers a confident approach to the customisation of the structural, morphological, and thermal features of ZnS nanoparticles. This work has provided important information to the existing literature on the synthesis of scalable and functional ZnS nanomaterials by directly relating synthesis conditions with functional outcomes.

## 9. CONCLUSION

This paper was able to show the process of synthesizing ZnS nanoparticles through a regulated chemical displacement pathway and showed a thorough analysis of their structural, morphological and temperature characteristics. X-ray diffraction studies described the development of a phase-pure cubic ZnS with nanoscale crystallite sizes, and electron microscopy described almost round nanoparticles with even size distribution and very little agglomeration. These findings suggest that the used synthesis plan is a successful method of controlling the nucleation and growth, resulting in structurally coherent and morphologically stable ZnS nanoparticles. Thermal analysis further defined that it has been synthesized that thermal stability of the ZnS nanoparticles is high, and this could be ascribed to the fact that they are highly crystalline, have a fine size of particles and low densities of defects. The fact that synthesis conditions are strongly related to thermal behavior indicates the efficiency of the chemical displacement method as a high-running and repetable method to manufacture ZnS nanomaterials with a high structural integrity. On the whole, this research provides interesting information regarding the process of synthesis by displacement and supports the significance of conditional optimization of high-performance semiconductor nanoparticles.

### *9.1. FUTURE WORK*

Further studies will involve his research to strategies of manipulation of the effective properties of ZnS nanoparticles by controlled doping of transition/ rare- earth elements to increase their optical, electronics and luminescent properties. Surface modification and functionalization strategies will also be addressed to enhance the dispersibility, interfacial compatibility and application-specific activities, especially in sensing and photocatalytic systems; the integration of chemically displaced ZnS nanoparticles into realistic device architects, including optoelectronic components, photodetectors and energy conversion systems, will also be explored in order to evaluate the real world performance and stability. Better-resolved in situ and time-

resolved characterization tools can be used to understand the processes of nucleation and the growth further and provide more advanced control over the processes and a wideness of the applicability of the chemical displacement synthesis methodology.

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