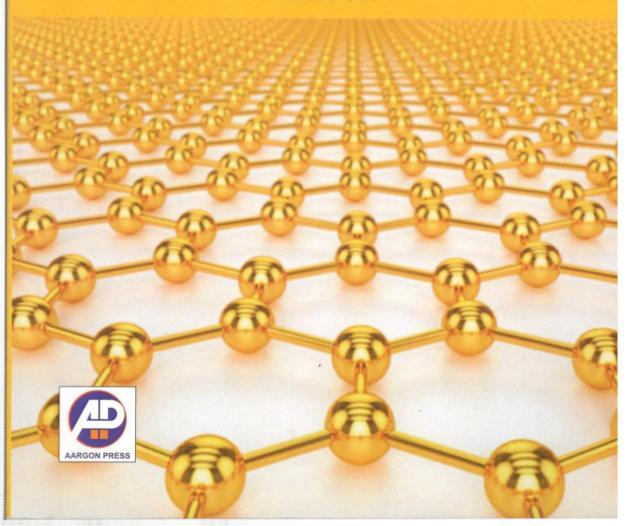


# Properties of Nanomaterials

Haroon



## **Properties of Nanomaterials**

#### **Editor**

Dr. Haroon

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# Synthesis and Characterisation of PANI-Ag-ZnO (Ag=3.0% and ZnO=0.1%) Nanocomposite

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Chemical oxidation was used to make polyaniline—silver and PANI-Ag-ZnO nanocomposites. The ZnO nanoparticles in the TEM scans are spherical, and the dark images reveal that they were solid. The homogeneous distribution of Ag and ZnO particles in the PANI matrix was revealed by TEM analysis of the PANI-Ag-ZnO nanocomposite. When FTIR spectra of PANI-Ag-ZnO composite were compared to those of pure PANI, the absorption peaks were observed to shift to a higher wavenumber. The interaction between the Ag, ZnO particle, and PANI molecule chains was blamed for the observed changes. The dielectric constant of PANI decreased following the production of PANI-Ag-ZnO nanocomposite, which is ascribed to the interfaces produced between ZnO nanoparticles and PANI, according to the dielectric research of PANI and PANI-Ag and PANI-Ag-ZnO nanocomposite.

Keywords: Nanomaterials, nanocomposite, Chemical oxidation, ZnO.

Nanotechnology is the manipulation of matter at an atomic and molecular scale that deals with materials, devices, and other structures with at least one dimension sized from 1 to 100 nm (1). Arising out of their size and surface-dominated properties nanomaterials exhibit unique optical, magnetic, electrical, and other emerging properties. Due to these important properties nanomaterials have a wide range of applications in the field of electronics, fuel cells, batteries, agriculture, food industry, medicines, etc (2). Nanofibers are important 1D nanomaterial that provides several amazing properties such as a very large surface area to volume ratio, high porosity, high gas permeability, small inter-fibrous pore size, flexibility in surface functionalities (3,4). Due to these outstanding properties nanofibers are used in many important applications, such as biomedical (5), electrical and

### Synthesis and Characterization of Pure Zinc Oxide and Cobalt Doped Zinc Oxide

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Zinc oxide (ZnO) and Co-doped ZnO nanoparticles were synthesized via the simple and economical Sol-Gel method. Forthe synthesis of pure zinc oxide, the process is based on the hydrolysis of Zn(CH<sub>3</sub>COO)<sub>2</sub>·2H<sub>2</sub>O and forthe synthesis of cobalt doped zinc acetate, the process is based on the hydrolysis of Zn(CH<sub>3</sub>COO)<sub>2</sub>·2H<sub>2</sub>O and Co(CH<sub>3</sub>COO)<sub>2</sub>·4H<sub>2</sub>O,heated at high temperature using distilled water as a solvent, NH<sub>4</sub>OH used as a medium for maintaining pH value.ZnO and Co-doped ZnO were characterized by XRD, FTIR, EDX, and SEM. X-ray diffraction results reveal that pureZnO has mainly zinc and oxygen peaks; which exhibits crystallinity in nature nanoparticles and Co-doped ZnO nanoparticles.

Keywords: Sol-Gel method, ZnO, Co-ZnO nano particle, XRD, SEM

Feynman introduced the concept of manipulation of matter at the atomic, molecular, and supermolecular levels. The golden era of nanotechnology began in the 1980s when Kroto, Smalley, and Curl discovered fullerenes and Eric Drexler of Massachusetts Institute of Technology (MIT) used ideas from Feynman's "There is Plenty of Room at the Bottom" and Taniguchi's term nanotechnology in his 1986 book titled, "Engines of Creation: The Coming Era of Nanotechnology."

Nanotechnology applications in the food industry include: encapsulation and delivery of substances in targeted sites, increasing the flavor, introducing antibacterial nanoparticles into food, enhancement of shelf life, sensing contamination, improved food storage, tracking, tracing, and brand protection (1). Nano food processing and products can change the color, flavor, or sensory characteristics; they also change the nutritional functionality, remove chemicals or pathogens from food.

# In-Situ Catalytic Growth and Characterization of CVD Synthesized Multiwall Carbon Nanotubes

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Carbon nanotubes were made using the Chemical Vapor Deposition process at temperatures about 800-1000°C, which is the ideal method for making carbon nanotubes since it allows for controlled growth and produces extremely porous nanotubes. The nanotubes were found to be very porous and tubular in structure using SEM. Nanotubes have a bandgap of 3.2 eV, indicating that they are semiconducting. The Particle Size Analyzer determined that the average width of produced nanotubes was 127 nm. Chemical sensors, field emission, near-field microscopy probes to scan the surface, and nano-electronics are just a few of the possibilities for these nanotubes. The uses of carbon nanotubes for different applications have been discussed.

Keywords: CarbonNanotubes, Chemical Vapor Deposition, Bandgap.

Carbon can exist in several allotropes and forms such as diamond, graphite, fibers, fullerenes, andnanotubes. Diamond and graphite have been well-known carbon materials for centuries. Carbon (from the Latin language, Carbo means coal) as a non-metal element can be found in every living organism; therefore, it can be bravely confirmed that the basis of one aspect of life is carbon. Carbon, as the original component presented in millions of various compounds, is capable of being very hard such as diamond or very soft as graphite. The use of this unique chemical element is almost unlimited from the hardest diamond for drilling to the softest form, graphite, for use as a lubricant in skin health and beauty. This nontoxic element is used as a filter to reduce other toxins. It has the highest melting point among all the known elements and occurs free in nature.

# Synthesis and Characterization of MgOand Zn DopedMgO Nanomaterial By Sol-Gel Method

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The optical and structural properties of MgO and Zinc doped MgO nanoparticles generated by the sol-gel process are reported. Sharp infrared peaks in pure MgO and zinc doped MgO confirm the Mg-O and Zn-MgO stretching vibrations, respectively. The XRD analysis shows that the produced MgO and Zn-MgO nanostructures have high crystallinity. MgO nanostructures created have an average crystallite size of 16nm, while Zn-MgO nanostructures have an average crystallite size of 18nm. Because of the increased ionic radius of Zn, the crystallite size of Zn-MgO is somewhat larger than that of pure MgO. The nanoparticle-based materials have distinct porosity architectures and positive surface charges, resulting in excellent adsorption capacity and efficiency.

Keywords: Nanomaterials, Sol-gel method, laser ablation method.

Whenever we think about nanoscience or nanotechnology, very small objects come to mind. Indeed, nanomaterials are expected to have a wide range of applications in various fields such as electronics, optical communications, and biological systems. These applications are based on factors such as their physical properties, huge surface area, and small size which offers possibilities for manipulation and room for accommodating multiple functionalities(1–5).

In recent years, major progress has been achieved in molecular electronics. As the physical limits of the conventional silicon chips are being approached, researchers are seeking the next small thing in electronics through chemistry. By making devices from small groups of molecules, researchers may be able to pack computer chips with billions of transistors, more than 10 times as many as the current technology can

### Synthesis and Characterization of Cu Doped NiO Thin Film by Spray Pyrolysis

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A simple and inexpensive spray pyrolysis method is used to deposit athin film on a glass substrate. The spray pyrolysis method, its advantages, and the deposition process are explained in this chapter. The experimental setup and substrate cleaning procedure are discussed indetail. The Chapter also includes a detailed explanation of precursor solution of different parameters in the set-up, preparation of precursor solution of doped and undoped NiO thin films, and also discussed the deposition process of pure and Cu doped NiO thin films.

**Keywords:** Thin films, spray pyrolysis, photoluminescence, physical vapor deposition.

During the last three decades, the chemical spray pyrolysis technique (SPT) has been, oneof the major techniques to deposit a wide variety of materials in thin-film form over aconsiderably large area(1-3). Spray pyrolysis is a process in which a thin film is deposited byspraying a precursor solution on a heated substrate; the solution is pulverized utilizing neutral gas so that it arrives at the substrate in the form of fine droplets. The substrate isgenerally kept at a high temperature where the constituents of the solution precursor react to form the desired chemical compound while other reaction products leave as volation of the contract of thelecomponents. The atomization can be done using a sprayer or atomizer (4). Fine quality thin films can be obtained by the optimization of deposition parameters viz, substrate temperature, concentration of the solution, nozzle to substrate distance, sprayrate, droplet size, and also the post-deposition cooling rate. The spray pyrolysis techniquehasbeen usedforthe preparation

ofthin films ofmetal oxides(4-6).

# Synthesis and Characterization of Plasmonic Gold Nanoparticles

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Gold nanoparticles have been of good use in medical and electronics applications due to surface plasmonic resonance. They can be used for catalysts, computing chips, nanomechanical parts, photo sensors, anovel platform for specific delivery of therapeutic agents, cosmetics, and ant-aging drugs. In this study gold nanoparticles have been synthesized by one shot wet chemical synthesis and seed-mediated synthesis. Optical properties have been studied by a UV-Visible spectrophotometer. Morphological and structural details were studied by SEM and TEM.

Keywords: Nanoparticles, plasmonic resonance, nano-spheres.

Elemental gold has many unique properties which have attracted and fascinated mankind since its discovery. Since the gold is very unreactive, hence it does not change in atmosphere and its attractive color of it remains forever (1). That is one of the main reasons for gold being used in shaping jewelry. It has been used for many colorful, decorative, ceremonial, and religious artifacts and has been a metal with a high monetary value. A Roman cup called the Lycurgus cup, used nanosized (ca 50 nm) gold and silver alloys, with some Cu clusters to create different colors depending on whether it was illuminated from the front or the back.

The cause of this effect was not known to those who exploited it. Michael Faraday was the first to recognize that the color was due to the minute size of the gold particles (2). On February 5, 1857, Michael Faraday delivered the Bakerian Lecture of the Royal Society in London entitled "Experimental Relations of Gold (and other metals) to Light". In his speech, he mentioned that known phenomena (the nature of the ruby glass) appeared to indicate that a mere variation in the size of its particles gave rise to a variety of resultant colors. Nearly a century later, electron microscope investigations

### Study of Nonlinear Optical Properties of Urea (NH<sub>2</sub>CONH<sub>2</sub>)

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Nonlinear optics (NLO) is that branch of optics that helps us to study light's behavior in nonlinear media. A nonlinear media is one in which the material's optical properties such as dielectric constant, polarization density (P), etc. respondnon-linearly to the electric field E of the light. This nonlinearity is usually observed at extremely high light intensities, which are usually provided by lasers. A major role is played by NLO materials in nonlinear optics and information technology and industrial applications are greatly impacted by these. NLO materials that show second harmonic generation are much more in demand over the past few decades because of technological importance in various fields such as optical communication, instrumentation and signal processing. Both theoreticians and experimentalists were greatly attracted to urea due to its nonlinear optical piezoelectric properties. Urea is one of the molecules which are used in the study of NLO properties of molecular structure. Urea is a very well-explored system for its NLO properties. However, it is less extensively studied using quantum chemical methods. In the present work, NLO properties of urea were calculated via a quantum chemical method using density functional theory. Two density functionals viz. B3LYP and wB97XD were employed in conjugation with the 6-31+G (d, p) basis set to study this system. Various NLO properties such as dipole moment, dielectric polarizability (a), and first dipole hyperpolarizability (β) of urea monomer, dimer, and trimer have been calculated. Results of various polymers were compared within the same as well as different functionals. It is observed that results calculated with the wb97DX are closer to the experimental values.

Keywords: Density Functional Theory, Urea, Dimer, Homo-Lumo gap.

Nonlinear optical materials have evolved slowly over the past 20 years. At

### Semi-EmpiricalstudyofK-DecoratedAluminumNitrideNanotube

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Semi-Empirical method calculations have been carried out using AM1 functional 3-21G basis set for the investigation of electronic properties of potassium decorated aluminum nitride nanotubes. The density of states and various other parameters have been calculated. The study reveals that the K-decorated AlN nanotube show Al-N bond polarization this opens a door for AlN nanotube stobeused as a suitable hydrogen storage device.

Keywords: Semi-

empiricalmethod, Nanotubes, Nanostructures, Alkaliatoms.

Many investigations on carbon, boron nitride-based materials such as nanotubes, fullerenes, metal-organic and inorganic complexes have been conducted to date. New materials and approaches for hydrogen storage have been studied to overcome poor hydrogen storage. The hydrogen storage capacities of nanostructures have been extensively studied (1-6) and have been observed that pristine nanostructures have inadequate hydrogenstorage capabilities at a widerange of temperatures and pressures (7, 8). The application of alkali, alkaline, and transition metals to decorate nanostructures for hydrogen storage has been discovered (9, 10). Metals can be decorated with nanostructures like carbon single-walled nanotubes and boronnitride to altertheir electrical properties (11-13).

Hereweuseasemi-empirical method to carry out the calculations using AM1 functional 3-

21GbasissetfortheinvestigationofhydrogenstorageoverHydrogen terminated K-doped Aluminum Nitride (AlNNT). Optimized structures

#### Electronic transport through N-coupled noninteracting quantum dots in series: Exact calculation

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An analytical expression for Green's function in Keldysh's formalism for a system of N-coupled quantum dot array between the source and the drain leads has been found. Based on exact Green's function expressions for the dc-current, differential conductance and density of states are also obtained. The effect of temperature, resonant coupling with the leads, and also the number of dots between the leads on the transport is studied. The increase in temperature causes a broadening of the peaks' width and a fall in their heights. The resonant coupling with leads modifies the DOS profiles of the DOTs causing the differential conductance to achieve the maximum value when the resonant coupling is the same as that of the interdot tunneling and causes the number of resonant peaks to reduce to a value less than the number of dots when resonant coupling with the leads is larger than the interdot coupling.

**Keywords:**Quantumdot,Single-electrontunneling,Keldyshnon-equilibriumGreensfunction.

Quantum dots, often termed artificial atoms, serve as versatile structures that can be used to probe the quantum behavior of electrons on the nanometer scale. In recent times, transport through quantum dots (QD) has been studied extensively both theoretically and experimentally (1, 2) leading to a better understanding of a multitude of underlying physical phenomena(3, 4) such as the Kondo effect (5, 6), Coulomb blockade (7, 8), negative differential conductance (9, 10), formation of molecular states (11, 12), etc. Double quantum dots (DQDs) are more promising compared to their single dot counterparts for applications such as quantum information processing, spintronics, quantum computation(13,14), etc. The connecting leads to the DQD system can be taken to be ideal leads with a constant