Chapter 4
Nano-Level Modeling

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ABSTRACT

This chapter discusses the designing and modeling of nanomaterials through different updated technologies. It also covers the chemistry behind the nanoparticles and their prominent properties, which are required for different applications, along with an overview of the history of nanoparticle creation and applications. But the basic discussion is about different physical, chemical, and biological techniques for nanomaterial designing and different and novel characterization approaches to find the morphological and chemical traits of the designed nanoparticles. It also discusses the methods that are cost effective and eco-friendly for developing different nanoparticles. Future scope of designing nanoparticles and how the availability of nanomaterial helps in coping with the energy depletion and utilizing minute particles in massive applications are also covered.

INTRODUCTION AND BACKGROUND

With the advancement of nanomaterial, the scientific industry enters in the new horizon of research, development and technology and brought remarkable revolutions in modern world, from the last few decades number of synthesizing nanoparticles increase by 25 folds because of their increasing demand in every field. Nanoparticles have application almost in every field of science from electronics, mechanics, agriculture, medicine and forensics etc. As the scientific industry revolutionized the demand of nanomaterial is increasing day by day. Incorporation of nano matters in forensic science field brought more potential revolution in field of forensic science. By engineering this nanomaterial according to its requirement, it can be employed from trace detection to macro level detection but somehow its modeling is precise way is necessary for its meaningful usage Because of its minute sizing it provide more tactful particularities of the evidence make more reliable investigation.

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The term 'nano' coined from Greek word 'nanos' which means 'dwarf' in the conference of International Union of Pure and Applied Chemistry (IUPAC) in the year of 1947 this prefix was embraced in order to explain one billionth (10^{-9}) part of a unit. (Schaming & Remita, 2015b; Joudeh & Linke, 2022). Nanoparticle is defined as the matter particle having atomic size range of < 100 nm. Nano dimension material have more definite properties and discrete ionic make up than bulk material which provide more reactive surface, mechanical, electrical and magnetic properties. Because of these properties nano matter can be mold into various structures like nano films, nanotubes and bulk nano material used for different purposes. Nanomaterials are synthesized using a variety of processes, but energy-intensive approaches and intricate methods are major barriers to their widespread usage. Various methods have been discovered for designing nanoparticles form which some of them we will discuss in this chapter.

Categorization of Nanomaterials

On the basis of shape, origin, size and optical properties nanoparticles are categorized into variety of groups and sub groups. With size reduction, atoms perform better near the surface and stimulate different interactions with their surroundings than they do in the bulk material form. Additionally, the material's electrical structure is changed by decreasing the size, producing unexpected quantum phenomena. Additionally, size affects mobility, which is important for biological and environmental processes and is predominantly governed by Brownian motion for nanoparticles. (Shrestha, Wang, & Dutta, 2020).

Generally, the nanoparticle-based material was divided into two categories on the basis of origin. First type is nature based, like bacteria, proteins and viruses and other sources like nanoparticles created by forest fires, volcanic eruptions, minerals, nanostructured crystals and many more, the other type is human based whether they synthesized unintendingly like nanoparticles produced by the power plants, combustion of diesel or gasoline, and incinerators, as well as those created intentionally using a specified production process (Schaming & Remita, 2015b).

Nanomaterials are also classified on the basis of dimensions like zero-dimension, one dimension, two dimension and three dimensions. This dimensional classification is based on definition that one or more than one extensions of nanomaterial lie within the nanoscale i.e., less than 100 nm (Wani et al., 2022).

Another type of stratification is compositional base. Different composition forms are found in different nan matters like carbon based, organic based, inorganic nanoparticles, bio based nanoforms and metallic and metallic oxide nanoparticles fall in this stratum (Ijaz, Gilani, Nazir, & Bukhari, 2020).

On morphological basis nanoparticles are also classed as isometric and inhomogeneous or scattered and agglomerate depending on homogeneity. This aggregation relies on the electromagnetic, magnetic, and surface charge characteristics of NPs. Different morphological forms of nano matters includes nanohooks, nanoplates, nanostars, nanorods, etc. (Yun, Nam, & Kim, 2020).

Nanoparticles: Solution for Today

Today the world is facing energy crises. Renewable energy resources are depleting every day to cope up with this matter nanoparticles provide a solution. Nanoparticles provide solutions for saving, generating and utilizing energy in appropriate and efficient ways like solar cells, thin film nanocomposite, thin film batteries, semiconductors, transistors, integration of conductive nanomaterial with polymers which enhance the energy generation capabilities.