

Investigating The Catalysis of Nano Particles in The Process of Simulating Carbon Nanotubes and CNTs

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Note: *The properties and characteristics of nanoparticles generally depend on their type and size, and they have so many applications in various industries that it is not possible to check all of them. All the properties and characteristics that are created in nanoparticles can be justified by two factors: the increase in surface area relative to the volume and the discretization of energy levels.*

By changing the size of nanoparticles, the distance between the energy levels in them changes. The smaller the size of the nanoparticles, the greater the distance between the energy levels, and the larger the size, the smaller the distance between the energy levels. This point makes it possible to adjust the distance between their energy levels by changing the size of nanoparticles in such a way that they absorb certain waves with specific frequencies. For example, the dimensions of nanoparticles of a certain type can be adjusted so that they absorb infrared, ultraviolet, radio waves, etc. A catalyst is a substance that changes the rate of a chemical reaction (increases or decreases) but does not participate in the chemical reaction itself. A factor that has a great influence on the quality and performance of catalysts is a variable called its specific area. The larger the area of a catalyst material, the better its catalytic properties.

The specific surface area of a catalyst is obtained using equation 1:

$$S = A/\rho V \quad (1)$$

This quantity is usually reported in units of square meters per gram and its value for commercial catalysts is between 100 and 400 square meters per gram. 100 square meters per gram means that 1 gram of this material has an area of 100 square meters.

Nanoparticles can also be used as catalysts due to their high surface area. Of course, catalytic properties also occur in certain dimensions like magnetic properties. In other words, nanoparticles usually have catalytic properties if their specific surface is between 100 and 400 square meters per gram. Therefore, among nanoparticles with a specific volume, a nanoparticle with a larger surface area shows better catalytic properties. An example of nanoparticles that act as catalysts where various substances are placed on their surface and chemical reactions are carried out. Apart from the mentioned cases, nanoparticles have many other applications in various medical industries (drug delivery, etc.), automobiles (anti-fogging windows, lightening the body, strengthening tires), electronics (making transistors), etc. The strength of carbon-carbon bonds gives carbon nanotubes amazing electronic properties. No previous material exhibits the extraordinary combination of mechanical, thermal and electronic properties attributed to them. However, their conductivity is what sets them apart. Multi-layered carbon nanotubes are the strongest materials that mankind has discovered so far in terms of electronic conductivity. The highest tensile strength or breaking strain for a carbon nanotube was up to 63 GPa, which is about 50 times more than the strongest conductors. Even the weakest types of multi-layered carbon nanotubes have multifold power in electronic conduction. These properties, along with the lightness of carbon nanotubes, give them great potential in applications such as aerospace. The electronic properties of the wall of carbon nanotubes are also extraordinary. It has high electrical conductivity (comparable to copper). It is particularly noteworthy that nanotubes can be metallic or semiconducting. The rolling action breaks the symmetry of the planar system and imposes a specific direction with respect to the hexagonal grid and the axial direction. Depending on the relationship between these axial directions and the unit vectors that describe the hexagonal lattice, nanotubes may behave electrically like metals or semiconductors, with some nanotubes having higher conductivity than copper, while others behave more like silicon. And there are possibilities of making nano electronic devices from multi-layer nanotubes of CNTs.

Conclusion :

The properties and characteristics of nanoparticles generally depend on their type and size, and they have many applications in various industries that it is not possible to check all of them. All properties and characteristics that are created in nanoparticles can be explained by the two factors of increasing the surface area compared to the volume and the discretization of energy levels.

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