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Predictive Exponential Modelling of Gold Nanoparticles Total Surface Area (nm^2) and Diameter (nm) with NanoCalc Application in Nanoelectronics.

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***Abstract*:** *An exponential model that clearly predicts the total exposed surface area of gold nanoparticles at the same nanoscale dimension has been developed with the adoption of a nano calculator application. Physico-chemical parameters of diameter (nm), solution concentration (µM), and volumes (ml) were simulated from a value of 1 to 10 with the generation of the respective total nanoparticle surface area (nm^2). The plot of the total surface areas (nm^2) against the diameters (nm) generates an exponential model (**$y=5.001e^{0.9216x}$**) and a correlation factor of **$R^2=0.9057$**. Hence, Gold nanoparticles can effectively synthesize and optimized for diverse applications especially in nanoelectronics.*

Keywords: Gold nanoparticles, exponential model, surface area, diameter, NanoCalc.

1.0 INTRODUCTION

Nanotechnology highlights technologies at a scale of 10^{-9} meters, with applications in material sciences, computer sciences, biotechnology, medicines, engineering, and pharmacy [1]. Nanostructures through amorphous and crystalline forms have garnered several attention globally with their applications commercially and motivated to various researches that were dedicated to the development of diverse nano-applications [1]. The transistors and other microelectronic devices are getting smaller with modern microelectronics. Distances between transistors and relevant switching components on the microprocessor are simplified with miniaturization, as quantum phenomenal is becoming pertinent [2]. Contemporary nanolithography processing technologies enable scaling down to or below 50 nm with a significant impact on efficiency Traditional semiconductor circuitry and new opportunities for quantum effects [2]. Regarding the distribution with charging impacts, the coulomb effects permit the control of each of the charging carriers in metallic components consisting of tunnel intersections at submicron dimensions. Single electronics (SE) has been assigned to this field [2] as gold nanoparticles with optical-electronic properties are frequently exploited to be used in high-tech applications like electronic conductors, sensory detectors, catalysis, biological and medical drug delivery, and organic photovoltaic [3]. Ligand-coordinated gold nanoparticles with the length scale of a few nanometers are goals of great importance for future technological research in nanoelectronics [4]. In particular, gold nanomaterials possess suitable chemical activity, as they can be functionalized with virtually any form of electron-donating biomolecules. [5]. Further than that, few of the specific features of metallic nanoparticles in particular are readily evident simply by observing the nature of the melting point whilst decreasing the size of bulk material to the size aggregate in nanometers[2]. As a matter of fact, larger quantities of gold are with a melting temperature of 1064^0C with the elemental property that is specified with the reduction in the size of the metal under study, the melting temperature repeatedly decreases, and gold nanoparticles with a level of about 2 nm displays a melting temperature around 200^0C [2]. Such a lower melting value may be caused by the ratio of surface atoms to internal atoms when the particle size is reduced. The stabilized nano atoms retain a smaller percentage of coordination and are much more active. The melting point thus illustrates the initiation of atomic migration that is approximately equivalent to that in the melted form [2]. This tends to suggest that theoretically, it is possible to achieve a melting range of gold that is equal to ambient temperature. An additional dimension of fundamental importance (electrical properties) is realized when the amount of complete gold particles is reduced [6]. Individual nanomaterials of the sizes within the limit of some nanometers possess an electronic property that correlates to an electronic intermediate system between both the bulk metal band structure and the distinct energy rate of particles with its typical maximum molecular orbitals occupancy (HOMO)–lowest unoccupied molecular orbital

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Gap (LUMO) [2]. With the shape range of approximately 2 nm or less, a singular particle can be classified with quantum dots [2]. An extensive example is the well-known schmid cluster **[Au55 (PPh3)12Cl6 ('Au55')]** that was characterized by a dimension of 1.4 nm [2]. The sequence has been successfully exploited since its invention, with an excellent evaluation of the compound [2]. Investigations into tunneling spectroscopy (STS) impedance spectroscopy (IS), and voltammetry revealed coulomb charging at ambient temperature [2]. This finding demonstrated that the compound is a beneficial constituent element in nanoelectronic components with the concept of Coulomb blockade with discrete charge regulated tunneling [2]. The ultimate underlying concept of nanoparticle synthesis is the reduction of metal salts by feasible reduction agents with the availability of ligands that generate auto assembled monolayers on the surface of the stabilizing agent [2]. In addition to the well-known citrate-stabilized gold nanoparticles and typical gold nanoparticles ligand molecules are thiolates, phosphine, and amines, due to their strong binding features with gold [2]. Citrate and sodium borohydride are also common reducing agents used in the direct reduction process [7]. The control over the particle size is usually accomplished by adjusting the ratio of ligand-stabilizer / gold salt. Without any apparent change in properties [2] the respective nanoparticles may be precipitated, dissolved, chromatographed, and further surface-modified. Therefore, to be able to envisage the manipulation of gold particles in terms of the total surface area with the diameter as the input factor, a model was designed using a nano-based application calculator.

2.0 METHODOLOGIES

2.1 NanoCalc application

This aimed at utilizing an android framework for measuring nanoparticles' chemical and physical parameters. By assigning the expected diameter and concentration of the nanoparticles, NanoCalc enables measurement of the exposed surface area, the volume and mass of the individual nanoparticles, the total count of nanoparticles, and the total occupied volume.

2.2 Simulation

Arbitrary gold nanoparticles diameters, solution concentrations, and volumes were numerically infixed with the application (Table 1).

3.0 RESULTS AND DISCUSSION

Table 1. Total Nano Gold simulated surface area

Data input			Data Output	
NPs Diameter (nm)	**NPs Solution Conc.(μM)**	**NPs Solution Volume (ml)**	**Total NPs Surface Area (nm^2)**	**Total NPs Surface Area(xE15) (nm^2)**
1	1	1	1.89E15	1.89
2	2	2	3.03E16	30.3
3	3	3	1.53E17	153
4	4	4	4.84E17	484
5	5	5	1.18E18	1180
6	6	6	2.45E18	2450
7	7	7	4.54E18	4540
8	8	8	7.75E18	7750
9	9	9	1.24E19	12400
10	10	10	1.89E19	18900

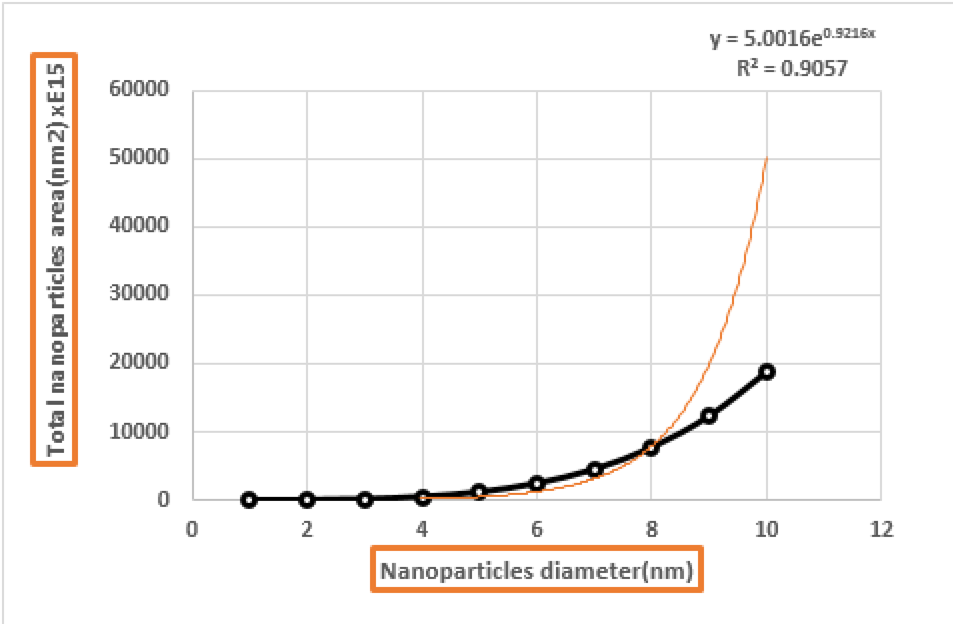

Figure 1. Exponential plots of Gold nanoparticle diameters against the total exposed area.

The simulated output is the total exposed surface area of the gold nanoparticles as expected under standard and atmospheric factors. Overtime gold nanoparticles have been extensively developed by a reduction of chloroauric acid. Once the acid is dissolved, the formulation is quickly blended with an agent of reduction. It then transforms the Au^{3+} ions to neutral gold atoms. The solution will become completely saturated as several of these gold atoms are obtained. Metallic gold subsequently starts to crystallize in the state of particles below the nanometer. When the nanoparticles solution is robustly mixed, they will be homogeneous in structure. Often a stabilizing entity is added to avoid aggregation of the particles .The generated model from the interaction of nanoparticle diameters and the total exposed surface area was purely exponential ($y=5.001e^{0.9216x}$) with a strong correlation ($R^2=0.9057$).

4.0 CONCLUSION

The gold nanocrystals are versatile materials that are traced to the well-designed synthetic methodologies and systematically characterized physical, chemical, and electronic properties for a broad range of applications. They are developed from printable inks to electronic chips for use as conductors. Because the electronics world is getting smaller, nanoparticles are critical elements in circuit designing. Moreover, their surface chemistry is easy to alter by the thickness, surface area, concentration, mass, and volume of its synthetic materials. All these characteristics have rendered gold nanoparticles as the extensively exploited nanoparticles for educational research as well as an essential aspect of industrial and medical breakthroughs globally. The vast array of gold metallic nanoparticles, available to the international scientific world intended to enhance their usage in high-tech engagement. Additionally, predictions can be made at the same level toward the physical, chemical, and morphological orientations of nanoparticle applications.

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