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COMPUTATIONAL NANO TECHNOLOGY AND SIMULATION TECHNIQUES APPLIED TO STUDY SILVER NANO DOTS

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Abstract: *In this report we study the computational nano technology methods and their applications. There are three distinct classification of nano technologies-1)wet nano technology,2)dry nano technology,3)computational nano technology. Complex processes takes place at the nano scale and new models of computation and analysis has to be developed and applied. Advancement in computer simulation and modeling is applied for better study and faster results such as1)faster algorithms2)optimization and predictability 3)complex nano structures and interfaces simulation 4)crossing time and length scales 5)dynamics, assembly and growth of nanostructures 6)well characterized nano building blocks at the molecular level and scale. Computational nanotechnology makes available the use of computer algorithms and techniques for the design of new nano devices*

Key Words: Computational modelling ,silver quantum dots,3D visualization, Quantum dot lab.

1. INTRODUCTION

In recent years ,intelligent and sophisticated computational tools have been developed to investigate and analyse "matter at the nano scale dimension" .So we find computational technology has led to the development of computational models of chemical and physical process systems which allow us to simulate various nano materials and applications. The advancement in this technical field has increased the computing power and 3D techniques enabling nano tech researchers to handle complex data at the nano scale molecular dimensions. Computational nano technology can be widely used in broad areas such as 1)Molecular modelling 2)Nano devices simulation 3)High performance computing 4)Nano informatics 5)Nano technology inspired computing.

2. METHODS OF STUDY

Hence the main aim of this study is to simulate silver nano dots with varying degrees of complexity and so we use the available models, soft wares and 3D techniques. Here in this study various soft wares were used such as Quantum dot lab and others .Computational simulation was used to analyze the silver nano dot structure. The structure of luminescent nano dots was studied and the results showed a charged core as Ag2+ or Ag5+.This observation establishes the fact the positively charged silver nano dots exhibit stability for longer time duration. The Quantum dot cellular automata simulator is used for the simulation of silver nano dots. The light emission on core shell dots and the pressure and temperature analysis in optical properties in a narrow band gap quantum dots can be studied.

QUANTUM DOT LAB analyses and computes the Eigen states of a particle in a box of varying shapes including pyramids and domes, cones, cuboids, spheroids, phonon spectra , coupled quantum dots systems. Users can choose between simple single band effective mass model, two band effective mass model and 10 band sp3 d53* tight binding model(with spin-orbit coupling) and run interactively.

3-D visualization depicts the 3-d confined wave functions. Optical transitions are computed and sorted into dark and light lines. Absorption curves are computed for different polarizations and orientations. The various parameters such as incident light angle, polarization, Fermi band, temperature can be modeled on this 3-d platform. The simulation is fully parallelized and depending on the device structure the tools decide the computational resource to be used and for simulation.

Molecular dynamics with fast multi pole methods for computing long-range inter atomic force have made accurate calculations possible on the dynamics of nano structures like silver nano dots ,nano wires and others. This time dependent modeling mimics the behaviour of molecules of nano dimensional systems. The movement of the atoms in a molecule is influenced by the atoms around it. This type of dynamic state can be well analyzed by differential equations. A molecular dynamics simulation starts giving some kind of kinetic energy to the atoms in a system. By using Newton's equations of motion one can solve and analyses the molecular motion of the particles .Also by analyzing the energy of the molecule and using this information we can predict what will happen in a short period of time forward. The entire chemical

process of the nano molecules can be studied. The package NANO MATERIALS SIMUALATION TOOL KIT analyses molecular process and simulation of nano materials. The molecular modeling techniques also use Hartree –fock methods but it is quite expensive. Density functional theory method is based on strategy of modeling electron correlation from electronic density functional. Computational algorithms based on this method is used for quantum mechanical simulated models. Also Quantum Monte Carlo methods now promise to provide nearly exact descriptions of the electronic structures of molecules and quantum nano dots. The Car-Parrinello method for ab initio molecular dynamics with simultaneous computation of electronic wave functions and inter atomic forces has opened the way for exploring the dynamics of molecules in condensed media as well as complex interfaces. Fast work stations, cluster computing and new generations of massively parallel computers complete the picture of theory, modeling and simulation. These hardware and software tools are continuing on the Moore's Law exponential trajectory of improvement ,doubling the computing power available on a single chip. The study of silver nano dot dynamics can be modeled by applying the latest simulation models and monte carlo techniques.

3. CONCLUSIONS

With the reduction in size up to the nano scale, quantum effects dominate. The properties of electrons in matter are influenced by variations in nano scale. It is possible to vary microscopic and macroscopic properties of the substance altering the configuration of nano materials by using these computational simulation techniques.. Therefore, it is possible to change the charge mobility, magnetic effects, melting point and other features without changing the chemical composition of the materials used. These computational nano tech methods make the study of silver quantum dots a lot more easier, faster and accurate.

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