College of Science
Department of Physics

M.Sc. Lectures
Semester I
Nano-physics

PROPERTIES OF INDIVIDUAL NANOPARTICLES

REF. INTRODUCTION TO NANOTECHNOLOGY BY POOLE, & OWENS

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PROPERTIES OF INDIVIDUAL NANOPARTICLES

Introduction

A nanoparticle is an aggregate of atoms between 1and 100nm viewed as a subdivision of a bulk material, and of dimension less than the characteristic length of some phenomena.

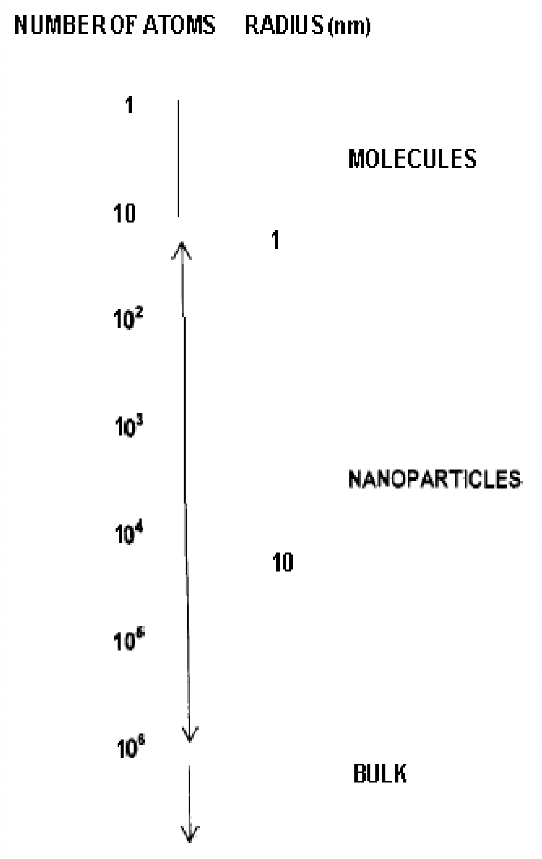
Because nanoparticles have 10^6 atoms or less, their properties differ from those of the same atoms bonded together to form bulk materials.

For example, a cluster of one nanometer radius has approximately 25 atoms, but most of the atoms are on the surface of the cluster.

This definition based on size is not totally satisfactory because it does not really distinguish between molecules and nanoparticles.

Many molecules contain more than 25 atoms, particularly biological molecules.

What makes nanoparticles very interesting and endows them with their unique properties is that their size is smaller than critical lengths that characterize many physical phenomena.
Generally, physical properties of materials can be characterized by some critical length, a thermal diffusion length, or a scattering length,



For example:
The electrical conductivity of a metal is strongly determined by the distance that the electrons travel between collisions with the vibrating atoms or impurities of the solid. This distance is called the mean free path or the scattering length. If the sizes of particles are less than these characteristic lengths, it is possible that new physics or chemistry may occur.

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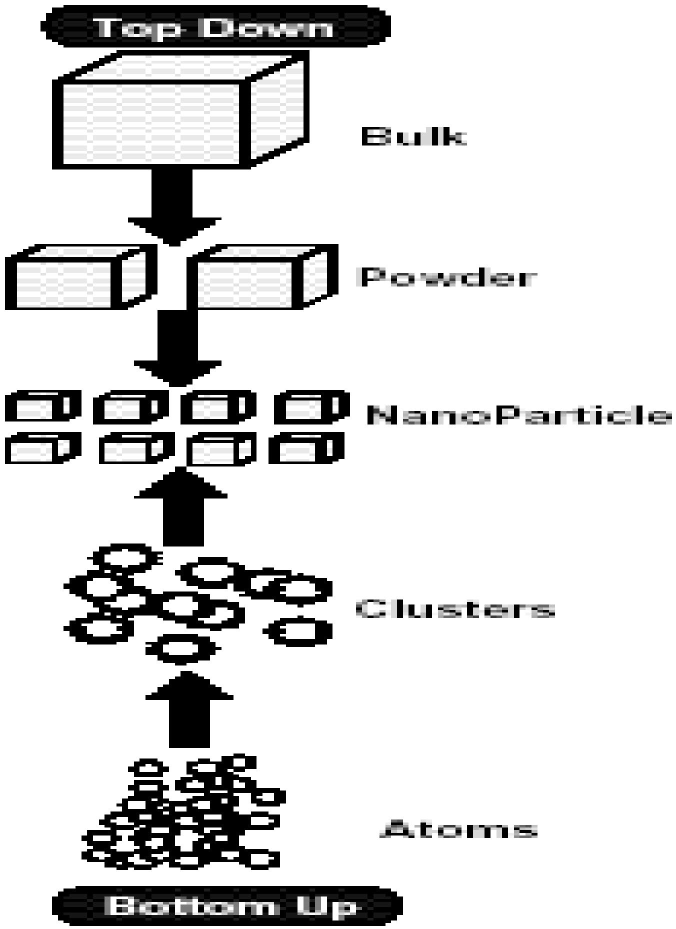

Top Down Methods

Mechanical Grinding

Erosion

Bottom Up Methods

Aerosol Techniques

Chemical precipitation

Gas phase agglomeration

Self Assembly

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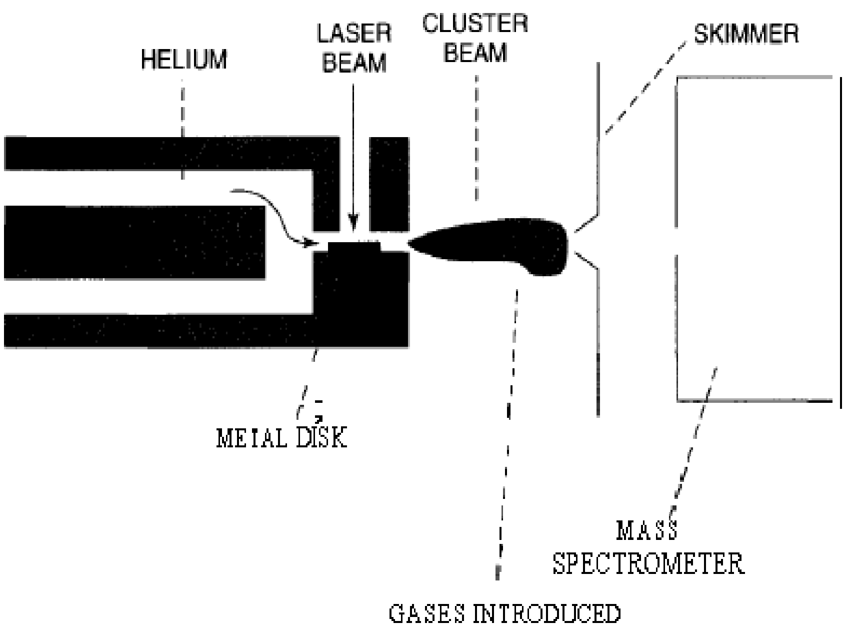
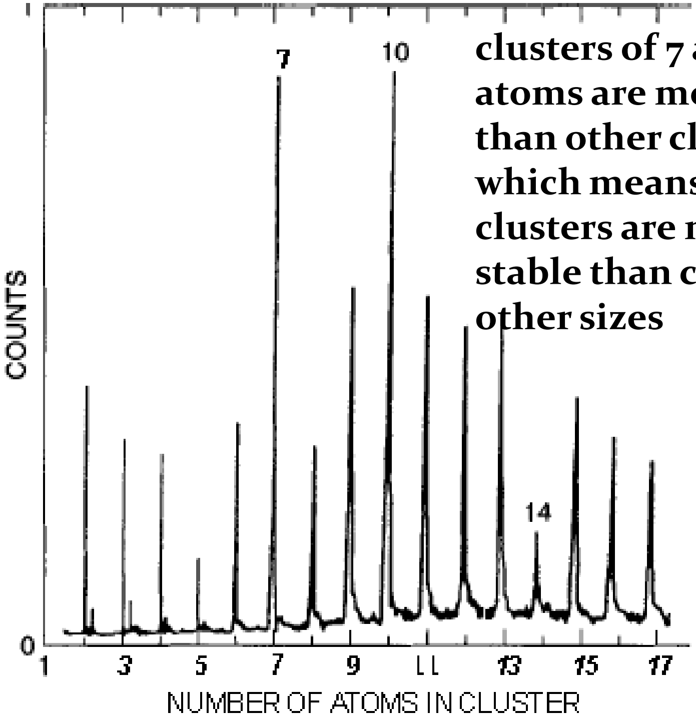
METAL NANOCLUSTERS

A <u>high intensity</u> **<u>laser</u>** <u>beam</u> is incident on a **<u>metal rod</u>**, causing <u>evaporation of atoms</u> from the surface of the metal.
The <u>atoms are then swept away</u> by a <u>burst of</u> **<u>helium</u>**
and
passed through an orifice into a vacuum where the expansion of <u>the gas causes cooling</u> and <u>formation of</u> **<u>clusters</u>** of the metal atoms.

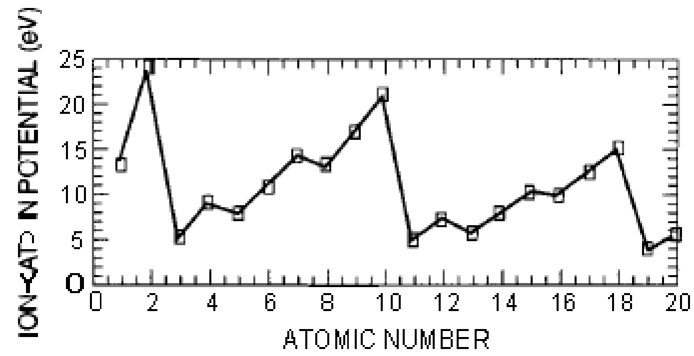


These clusters are <u>then ionized by</u> **<u>UV</u>** radiation and passed into a <u>mass spectrometer</u> that measures their (**mass :charge**) ratio.



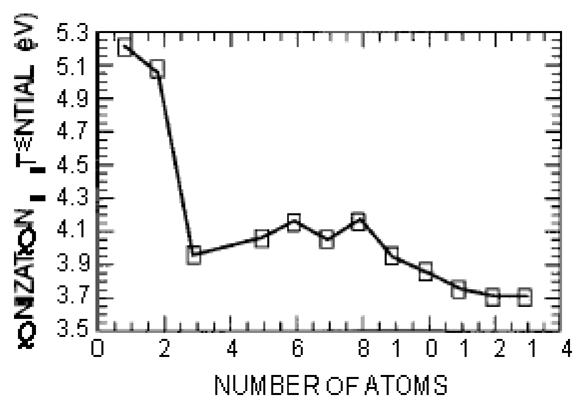
clusters of 7 and 10 atoms are more likely than other clusters, which means that these clusters are more stable than clusters of other sizes

The maximum ionization potentials occur for the rare-gas **atoms ^{2}He, ^{10}Ne, and ^{18}Ar** *because their outermost s and **p** orbitals are filled*.
More energy is required to remove electrons from filled orbitals than from unfilled orbitals



(a)

the mass spectrum data of lead clusters formed in such an experiment where the **number of ions** (**counts**) is plotted as a function of the **number of atoms** in the cluster

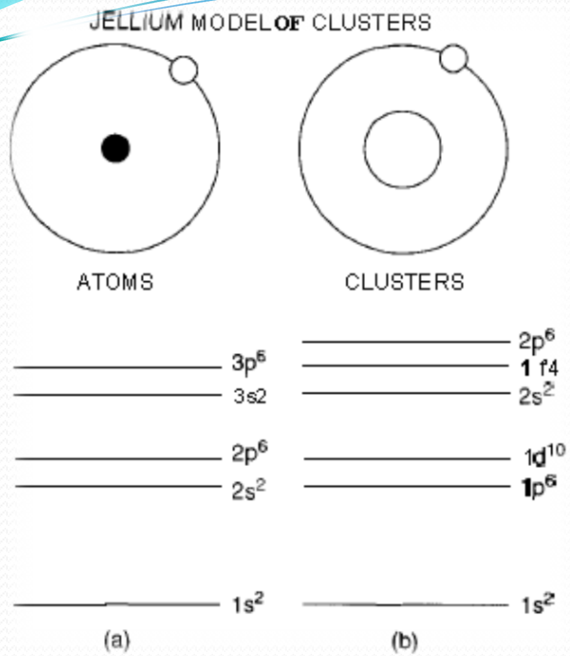


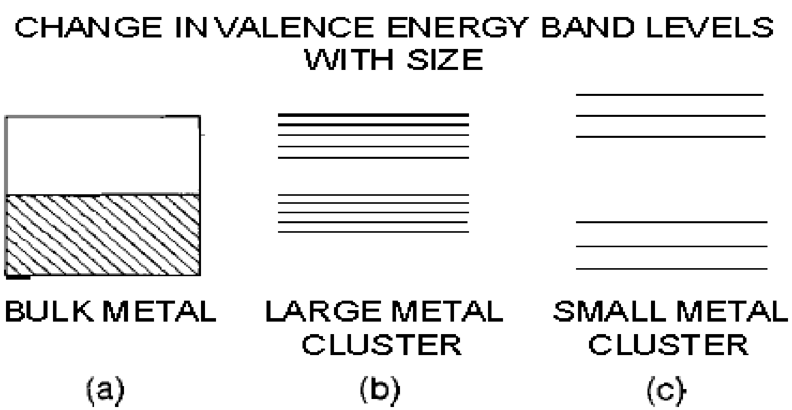
(b)

Their existence suggests that clusters can be viewed as **superatoms**, and this result motivated the development of the **jellium** model of clusters.

Figure b:
Peaks are observed at clusters having **two and eight** atoms. These numbers are referred to as electronic **magic numbers.**

Theoretical Modeling of Nanoparticles





The **jellium model** envisions يصور a cluster مجموعة عنقود–of atoms as a large atom.

The positive nuclear charge of each atom of the cluster is assumed to be uniformly distributed over a **sphere the size of the cluster**.

Thus the energy levels can be obtained by solving the Schrodinger equation for this system in a fashion analogous مشابهةto that for the hydrogen atom.

Figure , compares the energy level scheme for the hydrogen atom and the energy-level scheme for a spherical positive

The **electronic magic number** corresponds to the total number of electrons on the **super-atom** when the top level is filled. Notice that the order of the levels in the jellium model is different from that of the hydrogen atom. In this model the magic numbers correspond to those clusters having a size in which all the energy levels are filled.

Electronic structures of nanoparticles

1.Discrete energy levels: atom-like energy levels

2. Separation of energy levels increases with decreasing particle size.

Electronic Structure

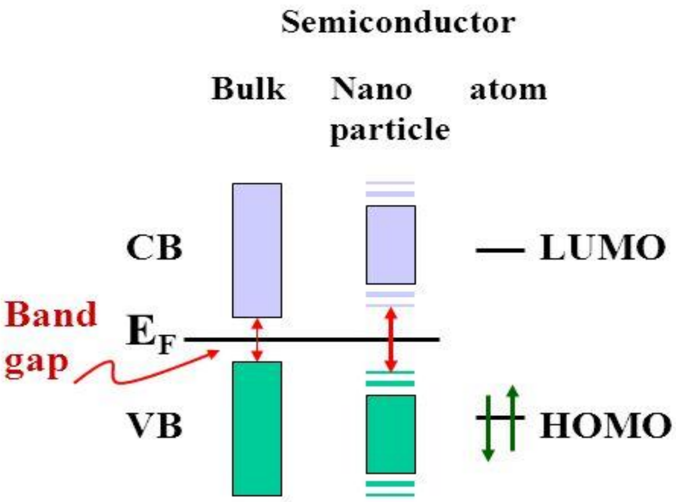
One method of studying the electronic structure of nanoparticles is UV photoelectron spectroscopy

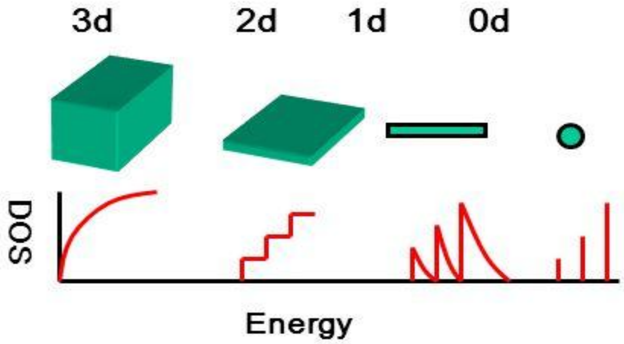
Eventually a size is reached where the surfaces of the particles are separated by distances which are in the order of the wavelengths of the electrons.

In this situation the energy levels can be modeled by the quantum-mechanical treatment of a particle in a box. This is referred to as the *quantum size effect*

*** The emergence of new electronic properties can be understood in terms of the Heisenberg uncertainty principle**
*** The average energy will not be determined so much by the chemical nature of the atoms, but mainly by the dimension of the particle**
*** It is interesting to note that *the quantum size effect occurs* in semiconductors at larger sizes because of the longer wavelength of conduction electrons and holes in semiconductors due the larger effective mass.**
(in semiconductor the $\lambda \sim 1\mu m$, whereas in a metal it is in the order of 0.5nm)

Size Effect: *Energy Levels and DOS*





Size controlled *band gap tuning*
Discrete Energy levels

Optical Properties

1. The color of a material is determined by the wavelength of light that is absorbed by it.
2. The absorption occurs because electrons are induced by the photons of the incident light to make transitions between the lower-lying occupied levels and higher unoccupied energy levels of the materials.
3. Clusters of different sizes will have different electronic structures and different energy-level separations