Abstract

It is well known that our modern life is highly dependent on technological devices. Without any advancement of research in the field of science and technology, it would not have been possible to develop highly efficient electronic, mechanical and optical devices like sensors, catalysts, micro memory chips, lasers, optical switches etc. For the improvement of robustness, functionality and efficiency of technological devices, one must understand various properties of different materials. With the knowledge of individual materials, one can think of modifying properties through the composition of different materials. In fact, there has been sustained progress on tailoring various properties for bulk materials with composition.

It has been discovered that material properties may be modified abruptly by reducing the dimension of a material. As the materials become smaller in size, the surface to volume ratio increases and therefore surface properties start playing a dominant role, consequently, the structural, electrical, mechanical and optical properties change dramatically. For instance, bulk silicon behaves as a semiconductor while silicon atomic wire becomes metallic, small gold cluster is very much reactive while bulk gold is not. Observations of different material properties at lower dimensions gave birth to the field of nanoscience which helped in the development of nanotechnology. Nanoscience deals with nanodimensional structures such as Nanotubes, Nanorods, Nanowires, Clusters and atomic sheet like Graphene and many others. For the preparation of advanced material with desired properties, we must understand the electronic, magnetic, catalytic, mechanical and optical properties of various nanostructured materials. It should be noted that experiments at the nanoscale are very expensive and therefore, it may not be affordable in finding out

material properties through trial and error of experiments. However, understanding of various properties of nanostructured materials through theoretical calculations may be useful. The interesting properties obtained through theoretical calculations may be verified by experiments. Thus theoretical calculations are desirable as it saves time, energy and expenses.

To understand different properties of nano structured materials theoretically, one has to solve the many electron systems. As the number of particles is of the order of 10^{23}, it is not possible to solve the system analytically. It is even difficult to deal with so many particles numerically because it demands huge computing time. However, various sensible approximations have been adopted to solve such systems under the density functional formalism for extracting various interesting properties.

As mentioned before there are several kinds of nanostructures of various materials. However it is not possible to study all of them in single endeavor. Therefore, we have studied a few such systems and presented in this thesis. First we consider the possible formation of one-atom thick chains on a semiconducting subtrate. If these atomic chains are found to be metallic in nature, they will be very much useful as interconnects in electronic devices. In our study silicon (001) is chosen as the semiconducting surface. As bare silicon surface has dangling bonds all over the surface, the deposited atoms are unable to stick on the surface in a regular fashion. So, the dangling bonds are first passivated with hydrogen atoms. This hydrogen passivated Si(001) surface reconstructs into various patterns such as 1×1, 2×1 and 3×1. Among these patterns, the 2×1 phase is the most suitable because this phase may be achievable easily in experiments. Therefore we consider this Si(001):2×1 as the surface of the substrate. The surface is then patterned by desorbing desired hydrogen atoms from the surface so that the metal gold atoms deposited on it prefer to bind at hydrogen desorbed places on the surface. Structures of gold atoms adsorbed on the surface are studied for various submonolayer coverages. Our study indicates that one atom thick metallic gold chains may be formed.

Nanowires of semiconducting materials are also important as bandgap materials because their bandgaps may be tuned with respect to their diameter. Furthermore

by introducing magnetic material into such nanowires, it may be possible to combine the electronic properties of a semiconductor with spin-dependent functionalities of a magnetic compound. These are called diluted magnetic semiconductor (DMS) material. They may be useful for application in spintronic devices. In this context, II-VI semiconductors are very much important as they have wide direct bandgap at room temperature. The magnetic atoms have high solubility in these II-VI semiconductors. Therefore, II-VI based DMS are potentially attractive for developing a new class of spintronic materials. In our study we have taken ZnTe nanowire as the semiconducting material. The bandgap of pristine ZnTe nanowire decreases with the increase of diameter. Mn atom is chosen as the magnetic dopant material in our study because it has half-filled d orbitals with magnetic moment $5\mu_B$. Then it is doped in the ZnTe nanowire at various concentration. In Mn-doped ZnTe nanowire the Mn atoms prefer to couple anti-ferromagnetically, though a half metallic ferromagnetic state is observed at a higher energy.

Apart from nanowires, nanotube structures are also important for their interesting properties. After the invension of carbon nanotube, there has been huge interest on tubular structures of carbon material. However, as the structure plays an important role, people explored the possible synthesis of nanotubular structures of other materials. The synthesis of nanotubes made of non-carbon materials include selenium, platinum and many others. Selenium is an important semiconducting material. It has wide applications in photocells, photographic exposure meters due to its high photoconductivity. The synthesis of selenium nanotubes motivates us to investigate its geometrical and electrical properties for various diameters. Various single walled achiral selenium nanotubes are considered in our study. In contradiction to the semiconducting nature of bulk selenium, the nanotubes show metallicity irrespective of their diameters. Another important electrical property namely work function of the nanotubes are calculated and it can be tuned by varying the diameters of the tubes. On the other hand nanostructured materials of platinum show excellent catalytic activities. Metal catalysts are widely used in commercially important reactions, including hydrogenation, naphtha reforming, isomerization reactions

and electrocatalysis involving H_2 and O_2 reactions in a fuel cell. In particular, we have studied the dissociation of hydrogen and oxygen molecules as well as oxidation of CO molecule using platinum nanotube as a catalyst. The results indicate that platinum nanotubes have good catalytic properties and can be effectively used in converting CO molecule to CO_2.

Finally we pay our attention to another interesting nanostructure, namely, nanocluster. Nanoclusters are important for their optical and magnetic properties. Considerable efforts have been devoted to study the magnetic properties of clusters since they are the ultimate nanoparticles where size can be controlled one atom at a time. Former studies showed that magnetic moments of the clusters are enhanced over their bulk value and non-monotonically decrease towards their bulk limit. We have studied bimetallic clusters composed of gadolinium and transition metal atoms. Gadolinium, a rare earth metal is ferromagnetic while a transition metal atom for example Mn is antiferromagnetic in the bulk phase. Clusters of these elements, however, share some common properties; both exhibit ferrimagnetic behavior and maintain magnetic moments close to their free atomic value. If these atoms can be coupled ferromagnetically by using Gd as a hetero-atom, the total magnetic moment of a $GdMn_x$ cluster may be rather large. However, our study reveals that, the coupling between Gd and Mn spins is antiferromagnetic while that between Mn atoms is ferromagnetic. Even though the net magnetic moments of the bimetallic clusters are not huge, the bonding between Gd and Mn atoms is stronger than that between the Gd atoms or Mn atoms, thus enabling the possibility of creating more stable magnetic particles. These stable magnetic nanoparticles may be used as building blocks for creating magnetic lattices.

In short, structural, electrical, catalytic and magnetic properties of some nanostructures which are important for practical applications are studied theoretically in this thesis.