Abstract of the thesis titled :

Ab-initio Investigations on Structural, Electronic, Transport and Optical Properties of Bimetallic Nano Structures such as Au-Pd, Au-Ag, Au-Pt

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The expansion of research in field of Nano materials have covered numerous fields. Such increasing interest stems from two main reasons, 1) At nano scale properties of materials depend on size, structure and local arrangement of atoms. This offers a tremendous opportunity to customize the properties of the materials. 2) The potential application of nano structures due to the continuous need for miniaturisation of electronic components. The onset of miniaturisation of electronic industry brought together the need of efficient and multifunctional small-scale devices and interconnects. The ultimately small electrical interconnect that one can imagine would be a single metallic chain of atoms, which is often referred as atomic chains. One dimensional structure also is good choice for gas sensors and detectors because of their high surface to volume ratio.

Atomic chains have been extensively studied theoretically and experimentally in past two decades. The primary aim of these studies is to examine possibility of chain formation and to study various properties such as structural, mechanical, electronic, magnetic, transport and optical properties. Most of the studies related to one-dimensional structures are carried out for single element one dimensional structures. Of specific interest are the atomic chains made up of noble metals for their lower reactivity, higher stability and the transition metals for their fascinating magnetic properties. Alloying is proven to be the most convenient route to enhance, alter and tune properties at bulk level. With no difference to nano level, alloying provides an additional degree of freedom to tune various properties. However, alloy atomic chains are not much explored as compared to pristine atomic chains. In view of this we took up the topic of bimetallic nano structures.

There are two main experimental methods for chain formation. One class consists of atomic chains realised either by depositing metal atoms on any surfaces, mainly, semiconducting chains or transition metal atoms chain deposited on variety of surfaces or atomic chains grown in interior of nano tubes. Another class comprises of atomic chains produced by narrowing a junction between two metal tips. In the present thesis we address the theoretical aspects of both of the above-mentioned class of atomic chains. Our aim is to carry out a systematic study covering important aspects of bimetallic atomic chains namely formation possibility, stability, structure and interplay of properties with varied compositions.

The experimental methods for formation of atomic chains are broadly classified into two categories. (a) Suspended chains by using breaking of point contacts. Chapter 3 and Chapter 4 deal with the atomic chains corresponding to this class (b) Formation of atomic chain by

atom manipulation on a substrate. Chapter 5 of this thesis deals with this class of atomic chains.

Our motive for the work presented in this thesis is to study the aspects of (i) Formation possibility (ii) Composition dependence of different properties of bimetallic atomic chains, for the methods mentioned above.

This thesis presents computational results of structure, electronic, transport and optical properties of bimetallic atomic chains of Au-Pd, Au-Pt and Au-Ag. The calculations were carried out using Density Functional Theory implemented computational code VASP.

This thesis comprises of six chapters.

In **Chapter 1** the introductory aspects of nano structures are addressed emphasizing the focus on one-dimensional structures. A brief review of the pioneering work on 1D structures is presented with the emphasis on theoretical aspects of early experiments and mentioning important results regarding atomic chains from the past studies.

Chapter 2 is dedicated to essential theory and computational methods. The computations reported here are carried out using computational code Vienna Ab initio Simulation Package (VASP). Theoretical concepts behind each computational tool incorporated in VASP are presented. For the sake of continuity and completeness this chapter in the beginning mentions the historic development of formulation and basics of DFT calculations.

Chapter 3 reports results and discussion of our study related to Linear atomic chains. The aim is limited to interplay of properties and composition of bimetallic chains. The results of structure parameters, magnetic, electronic and optical properties of four different compositions of LAC of Au-Pd, Au-Ag and Au-Pt are reported.

Chapter 4 comprises the results of stability, structure and electronic properties of bimetallic chains Au-Pd, Au-Pt and Au-Ag. Similar to chapter 3, this chapter also deals with the free-standing chains however the study conducted here is on different aspects of chain study. We address the question of possibility of chain formation and the most likely composition of bimetallic chain to occur in an experimental set up.

Chapter 5 deals with the atomic chains adsorbed on substrate. This chapter reports DFT calculations on structure and electronic properties of bimetallic chains of Au-Pd, Au-Pt and Au-Ag on two different substrates NiAl(110) and Cu(110).

The final conclusions are given in **Chapter 6**.