

Table of Content

List of Figures	XII
List of Tables	XV
Chapter 1	
Introduction: An overview of nanostructures and Atomic chains	16
1.1 History, Present status and Futuristic applications.....	16
1.2 One dimensional structures.....	17
1.3 Experimental Methodologies for atomic chains	22
1.3.1 Scanning Tunnelling Microscope	22
1.3.2 Mechanically Controlled Break Junction.....	23
1.4 A brief account of work done on Atomic chains.....	23
1.5 Outline of the thesis.....	28
Chapter 2	
A Review of Theoretical Methodology	29
2.1 Background	29
2.2 The Many Particle Solids	30
2.3 Wave Function Based Methods to Solve a Many Particle Problem.....	31
2.3.1 Born-Oppenheimer Approximation	32
2.3.2 Hartree Approximation	32
2.3.3 Hartree-Fock Approximation	33
2.4 Density Functional Theory	35
2.4.1 Hohenberg and Kohn Theorems	35
2.4.2 Kohn-Sham Equation	36
2.5 Exchange and Correlation Functional	38
2.5.1 Local Density Approximation	38
2.5.2 Generalized Gradient Approximation	39
2.6 Self-consistent calculations.....	40
2.7 Numerical Implementation of DFT.....	41
2.7.1 Boundary Conditions.....	41
2.7.2 Description of ions	42
2.7.3 Iterative schemes for calculating the Kohn–Sham ground state.....	43
2.7.4 Partial Occupancy and finite temperature methods	44

2.8 Optical Properties using VASP.....	46
Chapter 3	
Composition Dependence of Electronic, Magnetic and Optical Properties of Bimetallic Linear Atomic Chains of Au-Pd, Au-Ag and Au-Pt.....	49
3.1 Introduction	49
3.2 Methodology.....	52
3.3 Structural Parameters and relative stability of LAC	52
3.4 Magnetic Properties.....	55
3.5 Electronic Properties.....	56
3.6 Optical Properties	57
3.7 Conclusion	65
Chapter 4	
Stability, Structure and electronic Properties of Bimetallic Atomic Chains of Au-Pd, Au-Ag and Au-Pt	66
4.1 Introduction	66
4.2 Calculation Details.....	67
4.3 Results and Discussion	68
4.3.1 Structure and Stability	68
4.3.2 Electronic and Optical Properties	73
4.4 Conclusion	77
Chapter 5	
Effect of Substrate on Structural and Electronic Properties of Au-Pd, Au-Pt and Au-Ag atomic chains	78
5.1 Introduction	78
5.2 Computational Details	79
5.3 Results and Discussions.....	81
5.3.1 Structure and Stability	81
5.3.2 Electronic and Magnetic Properties.....	86
5.4 Conclusion	94
Chapter 6	96
Summary	96
References	101