Chapter 5

Effect of Substrate on Structural and Electronic Properties of Au-Pd, Au-Pt and Au-Ag atomic chains

This chapter is devoted to the class of atomic chains which are realised on a substrate. NiAl(110) and Cu(110) substrates are most commonly used substrates in order to make chains of noble metals and transition metal elements. Bimetallic chains of Au-Pd, Au-Ag and Au-Pt with an alternating arrangement of each atoms were placed on NiAl(110) and Cu(110) substrate. We compared the effect of two different substrates on structural parameters, interaction of chain atoms and interaction of chain atoms with the substrate.

5.1 Introduction

The theoretical and computational studies of nanomaterials aims mostly at the understanding of how material properties depend on the structures at atomic scale. Knowledge of interplay between structural, electronic, transport, and mechanical properties of atomic scale systems such as atomic chains, clusters, and nanowires makes it possible to manipulate different properties to design desired atomic scale devices.[115–119] As discussed earlier there are two main experimental approaches to manufacture 1D structures. One is formation of a suspended atomic chains using break junction experiments[10,27,38] and the other is manipulation of atoms on the substrate with the help of scanning tunneling microscope that make one to several atoms thick nanowires on the substrate[24,34,128–130,120–127]. Chapters 3 and 4 are dedicated to the suspended atomic chains formed in break junction experiment. This chapter relates to manipulation of atoms on substrate. For the case of chain formation on a substrate the pioneering work was demonstrated by Nilius et al[122] on Au and Au-Pd chains formed on NiAl(110) substrate which was followed by a series of theoretical studies to get insight into interplay between structure and electronic properties.[12,122–128,131,132]. Recently a series of detailed study of bond formation and charge transfer mechanism for monomers and atomic chains of transition elements had been reported by Miguel

A[126–128,132]. The latest report along these lines sheds light into change in structural and electronic properties of atomic chains on alloying them by a single atom impurity.[133] Apart from structural and electronic properties magnetism of chain is highly influenced due to the weak chain-surface hybridization.[129,130] For example free standing ferromagnetic Cr and Mn chains undergo the transition from ferromagnetic to antiferromagnetic coupling when they are supported on Pd(110), Ag(110), and NiAl(110) surfaces[129]. Among all the reports on atomic chains on various substrate we found two important aspects which are least explored. (a) The effect of substrate on the structural, electronic and magnetic properties of bimetallic chains. (b) The effect of alloying on the interactions between chain and substrate atoms.

Our study on free standing bimetallic atomic chains of Au-Pd, Au-Pt and Au-Ag revealed that free standing atomic chains of Au-Pd and Au-Pt are magnetic and the magnetic moment depends on number and arrangement of Pd and Pt atoms in the chains.[134,135] It has also been seen that the most stable free standing chain structures have zigzag geometry and exhibit metallic properties. Taking the study of free standing bimetallic chains further we investigated how the presence of substrate surface influences the electronic, structural and magnetic properties of chain. We considered two most widely and extensively used surfaces for absorption of heavy 4d and 5d elements, NiAl(110) and Cu(110) substrate.[12,24,25,34,122–125,136126,12926,137] This study aims to answer to what extend electronic, magnetic and transport properties of a bimetallic atomic chain are modified due to the interactions between atoms of chain and substrate. The chapter is divided into four sections: After the introduction and brief review of the research done so far on atomic chains absorbed substrate, details of computation are reported in section-5.2. Our computed results are discussed in section-5.3, while conclusions are presented in section-5.4.

5.2 Computational Details

Similar to previous two chapters, the calculations of the present chapter also used Projector-Augmented-Wave (PAW) potential[83]. The exchange-correlation interaction between electrons are included through spin-polarized GGA with the PBE functional.[88,108] The kinetic energy cut-off of a plane wave basis is set to 450 eV by a high accuracy convergence criteria of 1meV. The convergence test for Brillouin zone

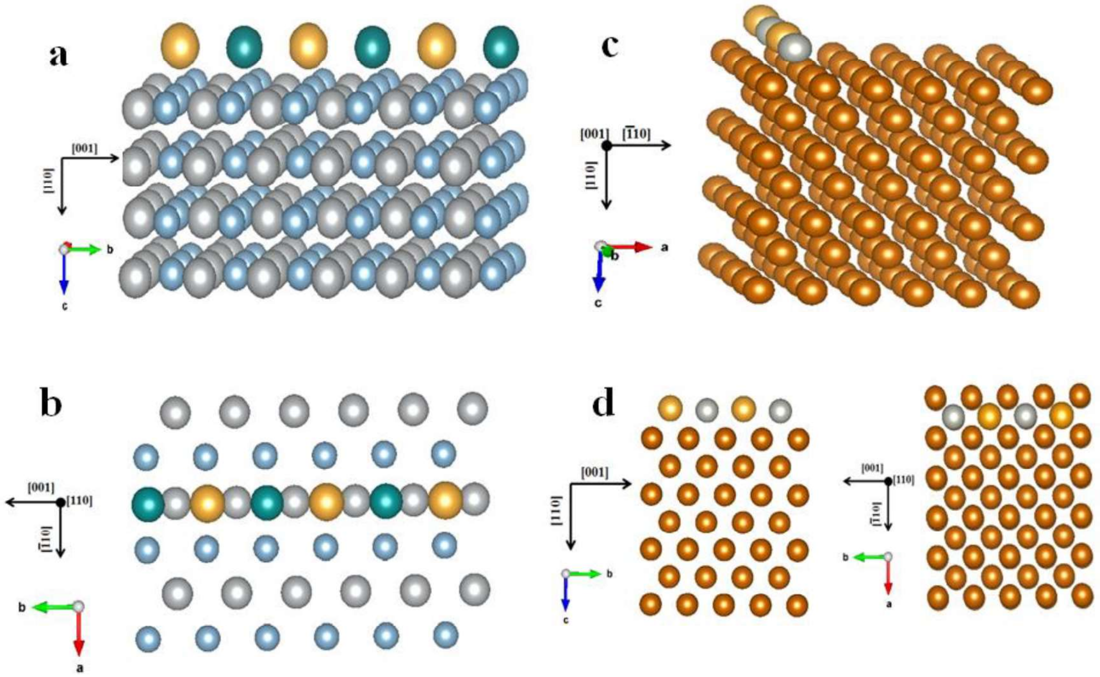

Figure 5.1: a) and b) Au-Pd, Au-Pt and Au-Ag chains over NiAl(110) substrate ; c) and d) Au-Pd, Au-Pt and Au-Ag chains over Cu(110) substrate. The copper atoms are represented by reddish yellow spheres. Al atoms are shown by light blue spheres while light grey spheres display Ni atoms in NiAl substrate. The chains atoms are shown by blue(Pd(Pt, Ag)) and yellow (Au) spheres, respectively, when are placed on NiAl(110) substrates. On Cu(110) substrate Pd(Pt, Ag) chain atoms are shown in grey color.

sampling for NiAl(110) and Cu(110) substrate yields mesh of 6x16x1 and 7x16x1 k-point mesh generated by the Monk horst−Pack scheme.[95] The partial occupancy was handled by method of Methfessel-Paxton using smearing parameter 0.1 eV. For obtaining accurate Density of States, tetrahedron method for smearing was considered. NiAl(110) substrate was modeled using four layers of (4×2) super cell. Cu(110) substrate was modeled using seven layers of (5×2) super cell. The chain axis was set along z-axis. A large vacuum of 20 Å along x-and y-direction was set to separate the chain from its periodic images. Bimetallic chains of Au-Pd, Au-Pt and Au-Ag are modeled having alternating arrangement of Au and Pd(Pt, Ag) atoms. Chain atoms are placed on NiAl(110) and Cu(110) substrate along [001] direction on Ni and Cu bridge sites which is the most favored direction for chain growth. In addition to single chains having alternate arrangements of atoms, geometry of copper substrate is favorable for placing two parallel chains. There are three possible ways to arrange any two of bimetallic chains on Cu(110) substrates which are termed as A, B and C and exhibited in Figure 5.1. The relaxed geometry corresponding to ground state of atoms is obtained by allowing all the atoms of the chains and first two layers of the substrate to change position in Conjugate Gradient minimization scheme Each chain/substrate system has been fully relaxed until the Hellmann-Feynman forces converged to a value less than 0.01 eV/Å per atom.

5.3 Results and Discussions

Substrate-chain(bimetallic) system is expected to have increased metal-metal interaction as compared to free standing bimetallic chains. With an aim to study the effect of increased metal-metal interactions on the structural, electronic and magnetic properties of chains on a substrate, we modelled two parallel chains of each of Au-Pd, Au-Pt and Au-Ag on the substrates of NiAl(110) and Cu(110). However, when two parallel chains are placed on the most stable Ni-bridge sites of NiAl(110) substrate, the distance between the two chains is found large for any noticeable interaction to occur between chains. For this reason, we restricted the modelling of two parallel chains to Cu(110) substrate only. Further, we found three possible configurations for arranging two bimetallic chains on copper substrate. These are displayed in the right panel of Fig. 5.2 and are termed as A, B and C types.

5.3.1 Structure and Stability

We first consider the case of single atomic chain on NiAl and Cu substrates.

5.3.1.1 Single chains on NiAl (110) and Cu (110) substrates

To study how presence of substrate influences the structural properties of bimetallic chains, we compare structural parameters of free-standing atomic chains with that of chains made on NiAl (110) and Cu(110) substrates.

From past studies it has been affirmed that the most favoured direction for growth of an atomic chain is reported to be the [001] direction on NiAl(110) surfaces and Cu(110) surface.[26,126–128,133,137,138] Considering the most favoured site for absorption of an atom on NiAl(110) surface, it has been found that Ni bridge site is energetically more favourable as compared to Al-bridge site.[126–128]. The reason is, Ni bridge sites on NiAl(110) surface provides a spacing of 2.89 Å along [001] direction for chain formation, which nearly matches with the nearest neighbour distance in bulk structures of Au, Ag, Pd and Pt.

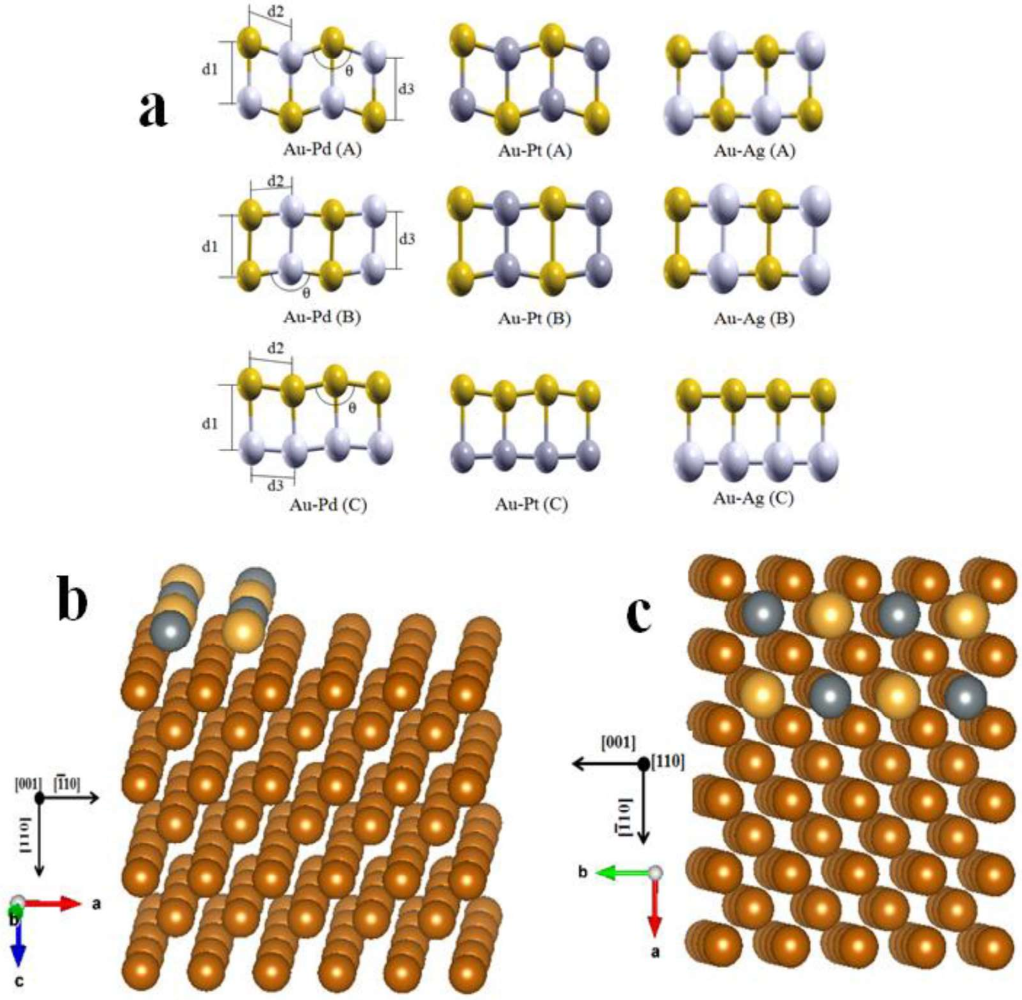

Figure 5.2: (a) Enlarged forms of chains without substrate are shown. Grey atoms represent Pd (Pt, Ag), while Au atoms are shown by yellow spheres. (b,c) Two different orientation of double chains placed on Cu (110) substrate. of Bimetallic chains placed on Cu(110) substrate. Relaxations of chain and substrate system yields three different possible configurations termed as A, B & C.

The nearest neighbour distances in bulk structures of Au, Ag, Pd and Pt bulk structure are 2.88 Å, 2.89 Å, 2.75 Å and 2.77 Å, respectively. On the other hand in case of Cu(110) substrate the available spacing for placing the chain atoms along [001] direction is 2.54 Å, which is not very different from interatomic distance for free standing linear chains of Au-Pd (2.50 Å), Au-Pt (2.51 Å) and Au-Ag (2.62 Å).[67]

Further, pristine chains of Au, Ag, Pd and Pt are known to make linear structures over the substrate.[128] Our computed results shows that bimetallic chains of Au-Pd, Au-Pt and Au-Ag do not exhibit linear structure when placed on NiAl(110) and Cu(110) substrate.

Table 5.1 Our computed inter atomic distances(d), bond angle(ɸ,θ), for the single chain placed on NiAl (110) and Cu(110) substrate respectively are reported here. Magnetic moment of free-standing chain (μ) is also listed in the table.

Chain Type	**$d_{\text{Al-Au}}$ (Å)**	**$d_{\text{Ni-Au}}$ (Å)**	**$d_{\text{Cu-Au}}$ (Å)**	**$d_{\text{Al-Pd (Pt, Ag)}}$ (Å)**	**$d_{\text{Ni-Pd (Pt,Ag)}}$ (Å)**	**$d_{\text{Cu-Pd (Pt, Ag)}}$ (Å)**	**Φ**	**θ**	**μ (μB /atom)**
Au-Pd	2.76	2.58	2.65	2.65	2.55	2.57	178°	174°	0.42
Au-Pt	2.80	2.59	2.68	2.58	2.54	2.53	173°	170°	0.62
Au-Ag	2.79	2.57	2.65	2.92	2.62	2.72	174°	175°	-

The bimetallic atomic chains over a substrate show a slight deviation from linearity and make a zigzag structure. The deviation is denoted by the angle Φ for NiAl substrate and θ for Copper substrate., which are reported in Table 5.1. The deviation from linearity can be attributed to the difference in atomic radii of alloy atoms, Au, Pd, Pt and Ag. This difference in atomic radii makes each of these atoms in alloy chain sit at different heights on the Ni or Cu troughs, which results into zigzag geometry of bimetallic chains.

Comparisons of the interatomic distance between chain atoms and substrate atoms along with interaction energy and PDOS give an idea about nature of bonding and comparative strength of the bonding. A shorter interatomic distance, higher binding energy and better orbital overlap indicates a stronger bond. Observing interatomic distance of chain atoms and substrate atoms from Table5.1, it can be said that Au-Pt chains bonds most strongly with the substrate compared to Au-Pd and Au-Ag chains. Stability of a structure is described in terms of Binding energy (E_B) and interaction energy of the structure. The E_B can be expressed as sum of two contributions coming from chain-substrate E_{C-S}, and chain-chain, E_{C-C} interactions. Thus; $E_B = E_{C-S} + E_{C-C}$, where

$$E_{C-S} = \frac{E_{tot} - E_{surf} - E_{adats}}{N_{at}} \tag{5.1}$$

$$E_{C-C} = \frac{E_{adats} - N_{at} \times E_{adats}}{N_{at}} \tag{5.2}$$

Our computed values of E_{C-S} and E_{C-C} for various chain configurations use of Eqns. (1) and (2) are reported in Table 5.2, which is given below:

Table 5.2 Computed values of E_{C-S} and E_{C-C} for single chains on NiAl (110) and Cu(110) substrates shown Fig. 5.1.

	E_B(eV/atom)	E_{C-S}(eV/atom)	E_{C-C}(eV/atom)
NiAl + Au-Pd	-3.55	-2.39	-1.17
NiAl + Au-Pt	-4.38	-2.88	-1.50
NiAl + Au-Ag	-2.88	-1.53	-1.35
Cu + Au-Pd	-3.43	-1.96	-1.47
Cu + Au-Pt	-3.86	-2.33	-1.53
Cu + Au-Ag	-2.79	-1.32	-1.47

As is seen from Table 5.2, the chain-substrate interaction energy (E_{C-S}) shows higher magnitude when NiAl(110) substrate is taken in place of Cu(110) substrate. The bond formation of Au-Pd, Au-Pt and Au-Ag atoms in the chains is stronger with Ni atoms of NiAl(110) substrate, as compared to that with Cu atoms in Cu(110) substrate. Further, among the three bimetallic chains, Au-Pt chains exhibit the highest magnitude of binding energy, followed by Au-Pd and Au-Ag chains for both the substrates. We find this consistent with the past calculations on single atom chains of Pt, Au, Pd and Ag made on NiAl(110) and Cu(110) substrates[126]. It is to note that the trend of chain formation in case of pristine free standing chain is highest for Pt followed by Au, Pd and Ag atoms.[40,71] Table 5.2 reveals the fact that all bimetallic single chains except Au-Ag chains on Cu(110) substrate show smaller magnitude of E_{C-C} than that of E_{C-}

S, suggesting a stronger interaction between atoms of chain and substrate, rather than interaction between the atoms of a chain. Another important observation that can be made from table 5.2 is that bimetallic chains bind more strongly with NiAl (110) substrate than that with Cu(110) substrate.

5.3.1.2 Double zigzag Chains on Cu (110) Substrate

This section reports results of structure and energetics for a system of two parallel chains of Au-Pd, Au-Pt and Au-Ag placed over copper substrate. As is shown in Fig.5.2, two single chains can be placed on copper substrate in three different manners. We found that after relaxation of chain-substrate system the geometry of the chains emerges to double zigzag structures or ladder structure, depending on the configuration of atoms, which are depicted in the Fig. 5.2.

The interatomic distances d_1, d_2 and d_3 and the bond angle θ, which characterize the equilibrium geometries shown in Fig.5.2, are reported in table 5.3. The d_1 and $d_3$denotes the distance between atoms of two different chains, while d_2 represents the distance between atoms of the same chain.

The distance between chain atoms of the same chain on Cu bridge site is of the order of supercell parameter 2.54 Å making the inter atomic distance d_2 for most of the chains same. However d_2 values are larger than 2.54 Å (<2.64 Å) for A-type structures of Au-Pd(2.64 Å) and Au-Pt(2.63 Å). This increased value of d_2 is responsible for the double zigzag geometry of the A-types of Au-Pd and Au-Pt chains over Cu(110) substrate as can be seen from Fig. 5.2.

Table 5.4 reports computed values of E_B, $E_{C\text{-}C}$ and $E_{C\text{-}S}$ for double zigzag structure chains over Cu(110) substrate. As is seen from the table, chain atoms bind most strongly with the substrate in case of Au-Pt and the most weakly for Au-Ag. Also, binding of chain-chain atoms is stronger than chain-substrate atoms. The observation of binding energies of all the three chains Au-Pt, Au-Pd and Au-Ag follows the trend; type-A>type-B>type-C suggesting that the type-A structure is most stable.

Table 5.3 Inter atomic distances(d_1, d_2 & d_3), and bond angle (θ), for double zigzag chains on Cu(110) substrate , which is exhibited in Fig. 5.2.

	d_1 (Å)	d_2 (Å)	d_3 (Å)	θ	μ (μB/atom)
Au-Pd (A)	2.78	2.64	2.78	148°	0.23
Au-Pd(B)	2.90	2.55	2.71	170°	0.05
Au-Pd(C)	2.74	2.56	2.55	163°	0.23
Au-Pt(A)	2.81	2.63	2.81	150°	0.41
Au-Pt(B)	3.12	2.56	2.61	166°	0.08
Au-Pt(C)	2.77	2.56	2.54	167°	0.09
Au-Ag(A)	2.84	2.54	2.84	178°	-
Au-Ag(B)	2.84	2.55	2.91	170°	-
Au-Ag(C)	2.90	2.54	2.54	179°	-

5.3.2 Electronic and Magnetic Properties

Analysis of projected density of state (PDOS) plots reveals strength of bond. Stronger covalent character of the bond is reflected in major overlap of orbitals. Our computed PDOS of bimetallic chains on NiAl and Cu substrates are plotted in Figures 5.3 to 5.6. These figures also exhibit the PDOS for free standing chains of Au-Pt, Au-Pd and Au-Ag.

On comparing PDOS of chain over substrate with those of free-standing chains, it is seen that the PDOS, which are confined to narrow energy range with higher peak values in case of free-standing chain, are transformed to those that have enlarged energy range and smaller peak heights when chains are formed on the substrates. This suggests that the 1D character observed in electronic properties of free-standing chains tend to be quasi-1D when chains are placed over the substrate.

Table 5.4 Computed values of $E_{C\text{-}S}$ and $E_{C\text{-}C}$ for double zigzag chains/Cu(110) system as exhibited in Fig. 5.2.

	E_B(eV/atom)	$E_{C\text{-}S}$(eV/atom)	$E_{C\text{-}C}$(eV/atom)
Cu + Au-Pd (A)	-3.49	-1.51	-1.98
Cu + Au-Pd (B)	-3.45	-1.55	-1.89
Cu + Au-Pd (C)	-3.41	-1.43	-1.98
Cu + Au-Pt (A)	-4.25	-1.73	-2.52
Cu + Au-Pt (B)	-4.23	-1.63	-2.60
Cu + Au-Pt(C)	-4.19	-1.68	-2.51
Cu + Au-Ag(A)	-2.81	-1.06	-1.75
Cu + Au-Ag(B)	-2.81	-1.13	-1.68
Cu + Au-Ag(C)	-2.78	-1.12	-1.66

Also, there is significant reduction in orbital overlap in atoms of chains when chains are placed on substrate compared to free standing chains. This reduction in overlap of atomic orbitals indicates weakening of bond strength between chain atoms. In case of chain on substrate, interaction of chain atoms with substrate atoms are found stronger, as compared to that between atoms of chain.

Further, we find that the magnetic moment observed in free standing chains of Au-Pt and Au-Pd is not seen when these bimetallic chains are formed on NiAl(110) and Cu(110) substrates. The transition to non-magnetic state in presence of substrate can be understood from two changes that are reflected in DOS plot: (i) Shifting of d-band edge away from Fermi level, and ii) stronger interaction of Pd/ Pt atoms in chain with the Ni/Cu atoms of the substrate, as compared to interaction between Au and Pd or Au and Pt atoms. Shifting of d-orbital away from Fermi energy in chain-NiAl system lowers the total density of states at Fermi level and neutralize spin polarization originated from reduced dimension of Pd and Pt d-orbital.

The discussions about PDOS plots of single chains on NiAl(110) and Cu(110) substrate and of PDOS plots of double zigzag chains on NiAl(110) and Cu(110) substrate are given below:

5.3.2.1 Single chains on NiAl (110) and Cu(110) substrate

Figure 5.3 compares PDOS of single chains of Au-Pd, Au-Pt and Au-Ag on NiAl(110) and Cu(110) substrates with that of free standing chains. First we compare orbital overlap of Au-Pd and Au-Pt chains on NiAl(110) and Cu(110) substrate. From Fig. 5.3, it is seen that Pd and Pt atoms show larger overlap of orbitals with the NiAl(110) and Cu(110) substrate atoms. Particularly Pd atoms of Au-Pd chains placed on NiAl(110) substrate show highest overlap with Ni atoms while Au atoms show negligible overlap with Ni and Al atoms. On the other hand, for the case of Cu(110) substrate, Au and Pd atoms shows good overlap with the substrate atoms. Next, we compare PDOS of Au-Ag chains in presence and absence of the NiAl(110) and Cu(110) substrate. It is clearly seen that Au and Ag atoms of the Au-Ag chains have good orbital overlap in presence of NiAl(110) and Cu(110) substrate while free standing Au-Ag chains exhibit small orbital interaction suggesting that presence of substrate enhances Au-Ag chain formation possibility.

As was discussed earlier in Chapter 3, free standing chains of Au-Pd and Au-Pt are magnetic and magnetic moment depends on interatomic distance. To find the effect of substrate on the magnetism of a chain, spin polarized calculation are performed for Au-Pd and Au-Pt chains in presence and absence of NiAl(110) and Cu(110) substrate.

It is observed that the presence of substrate, free-standing chains are non-magnetic. The magnetic moment per atom of free-standing single chains of Au-Pd and Au-Pt are reported in Table 5.1. Here it is important to notify that the purpose of magnetic calculation was to compare magnetism in presence and absence of the substrate.

Therefore, the magnetic moments of the chains, in absence of the substrate, is not computed for the ground state of the freestanding chains but it is computed with the same interatomic distance, as is in the chains on the substrate, which is larger than the ground state interatomic distances. The magnetic moment corresponding to ground state of free-standing chains is reported in Chapters 3 and 4.

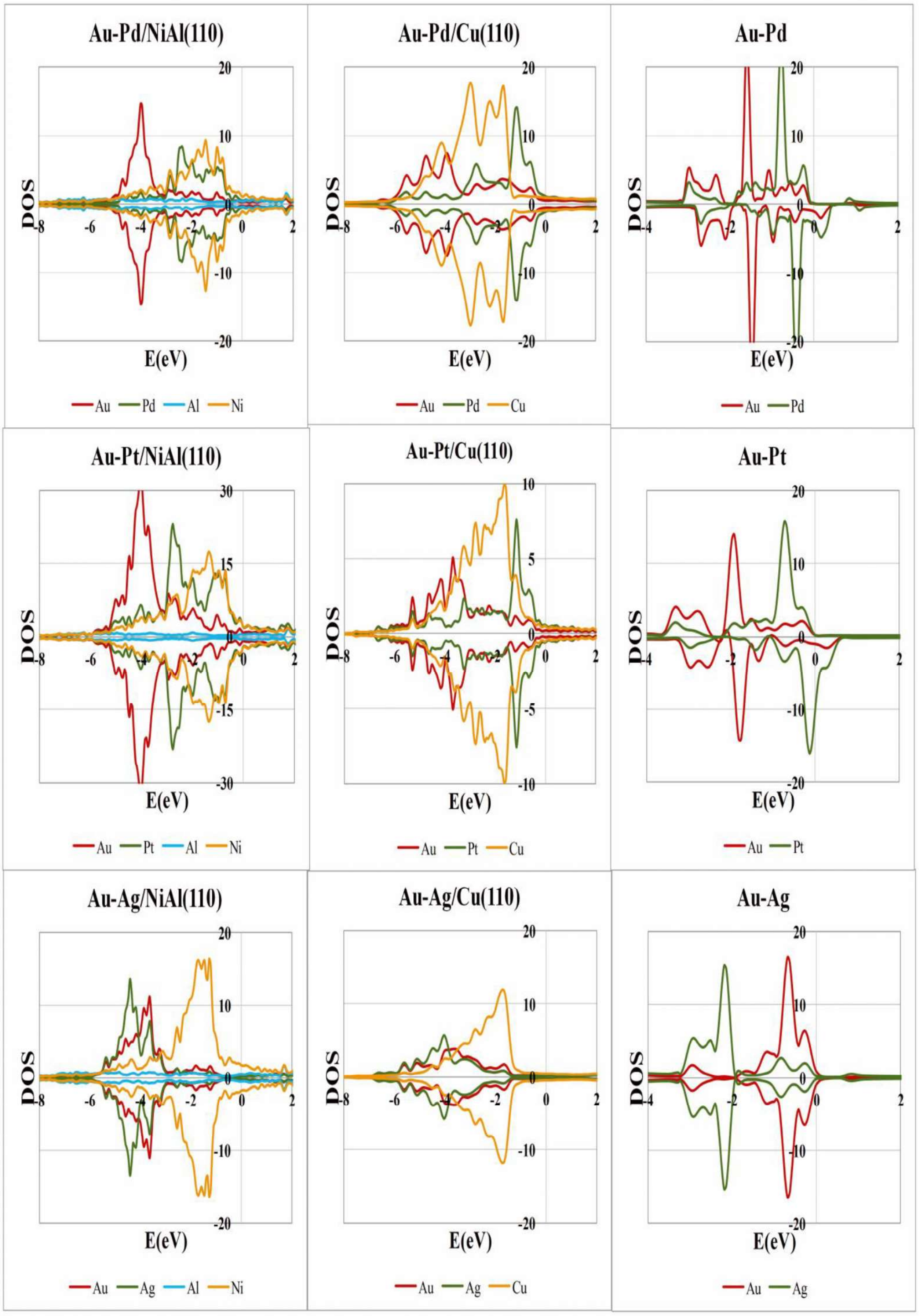

Figure 5.3: Projected density of states (PDOS) are plotted as function of energy for chain-NiAl(110), chain-Cu(110) systems. The PDOS for free standing chains of Au-Pd, Au-Pt and Au-Ag are also displayed in the figure.

5.3.2.2 Double zigzag chain on Cu (110)

Figures 5.4 to 5.6 display PDOS of Au-Pd, Au-Pt and Au-Ag chains, respectively, on Cu(110) substrate for three different configurations (A, B & C) that are shown in Fig.5.1. Similar to case of single chains, a refitting of PDOS from fermi energy is observed when double zigzag chain structures are placed on copper substrate. This refitting of PDOS reduces number of states near the Fermi energy for the chain substrate system as compared to free standing chains.

It is interesting to note that PDOS of A, B and C configurations are significantly different from each other which is not the case for binding energy, as binding energies of all these structures did not have a dramatic difference.

Fig 5.4 exhibits PDOS of three types of Au-Pd chain configuration on Cu(110) substrate. As is noticed from the figure, type-C structures show higher overlap of orbitals as compared to types A and B configuration. This trend is very different from that observed in case of free-standing chains, where orbital overlap of Au and Pd (Pt, Ag) atoms are found larger in type-A; followed by type-B and type-C configurations. This means that in case of free-standing chains type-A shows highest degree of alloying and in presence of substrate the highest degree of alloying is found for type-C configuration.

Figure 5.5 exhibits PDOS of Au-Pt chain in presence and absence of Cu(110) substrate. The trend of bonding of Au-Pt chain atoms on Cu(110) follows trend of Au-Pd chains where type-C configuration shows highest overlap of chain atoms.

Next, we compare the bonding between chain-substrate atoms as opposed to chain-chain atoms. From PDOS it is seen that Au-Pd, and Au-Pt chains possesses stronger chain-substrate bonding compared to the chain-chain bonding. While Au-Ag chain atoms prefers bonding more strongly with the chain atoms rather than substrate Cu atoms.

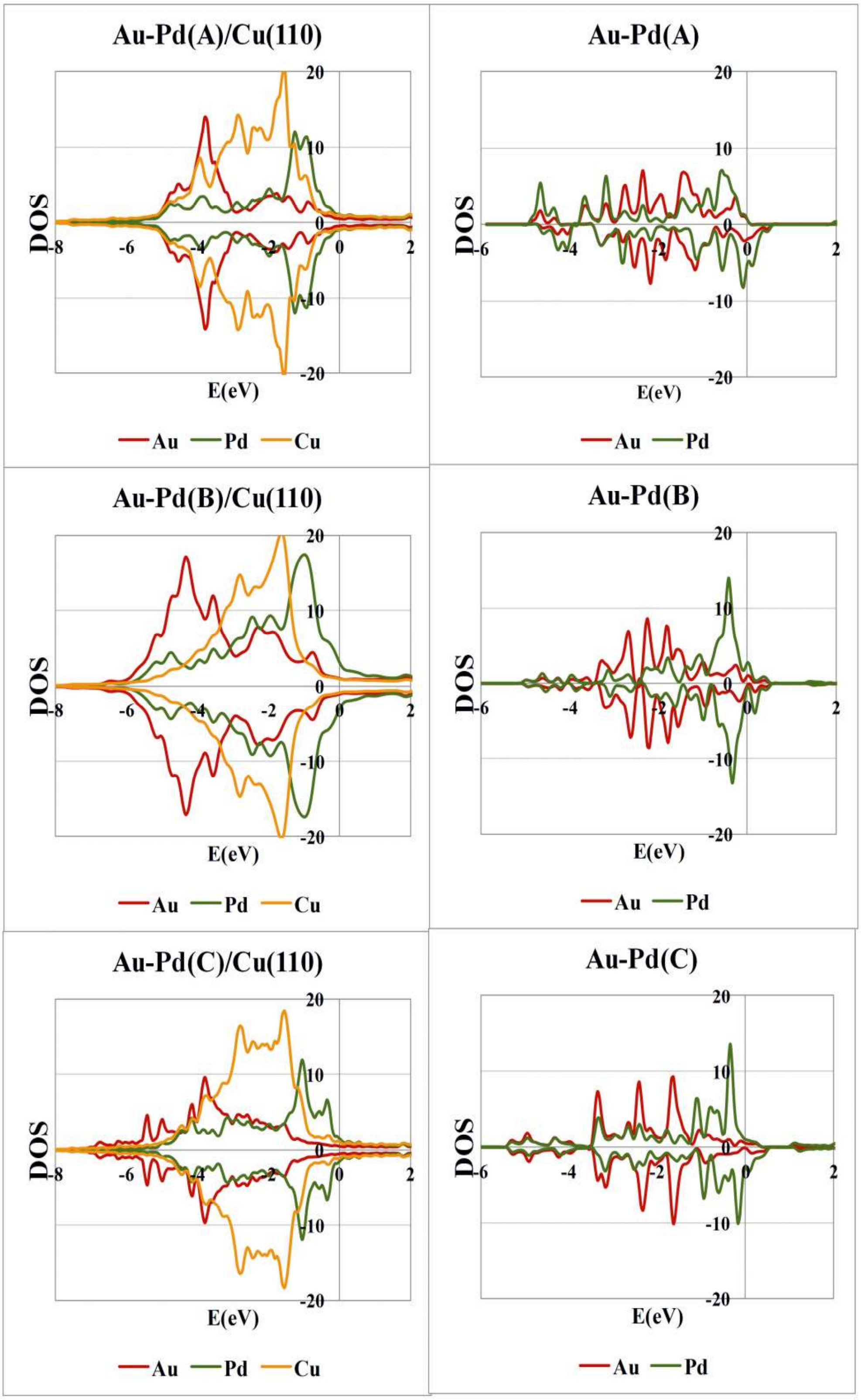

Figure 5.4: PDOS for different configuration of Au-Pd double zigzag chains on Cu (110) substrate (left panel) and corresponding free-standing chains of Au-Pd(right panel). The structures are exhibited in Fig.5.2.

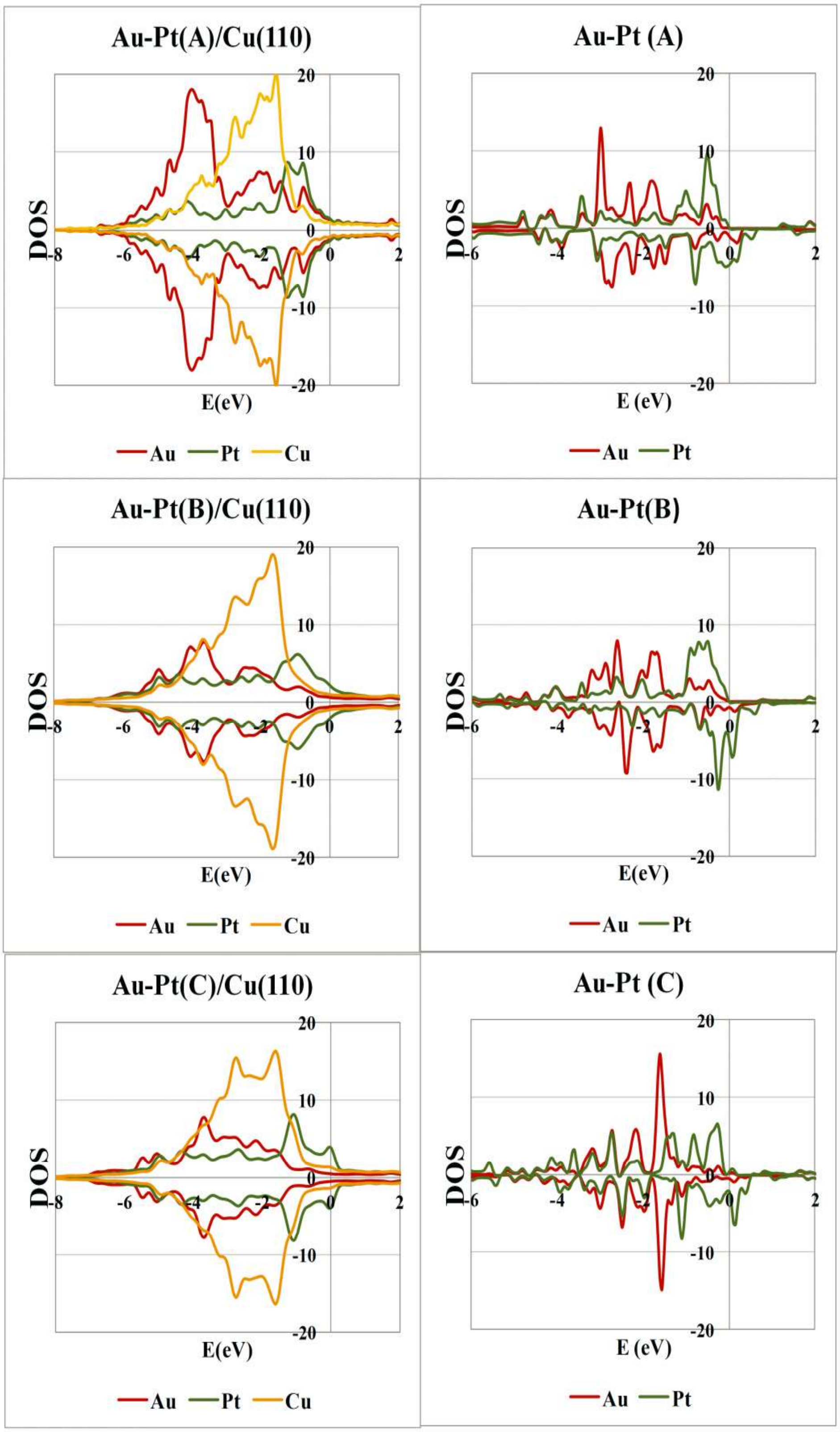

Figure 5.5: PDOS for different configurations of Au-Pt chains on Cu (110) substrate (left panel) and for corresponding free-standing chains of Au-Pt(right panel), whose geometries are as shown in Fig. 5.2.

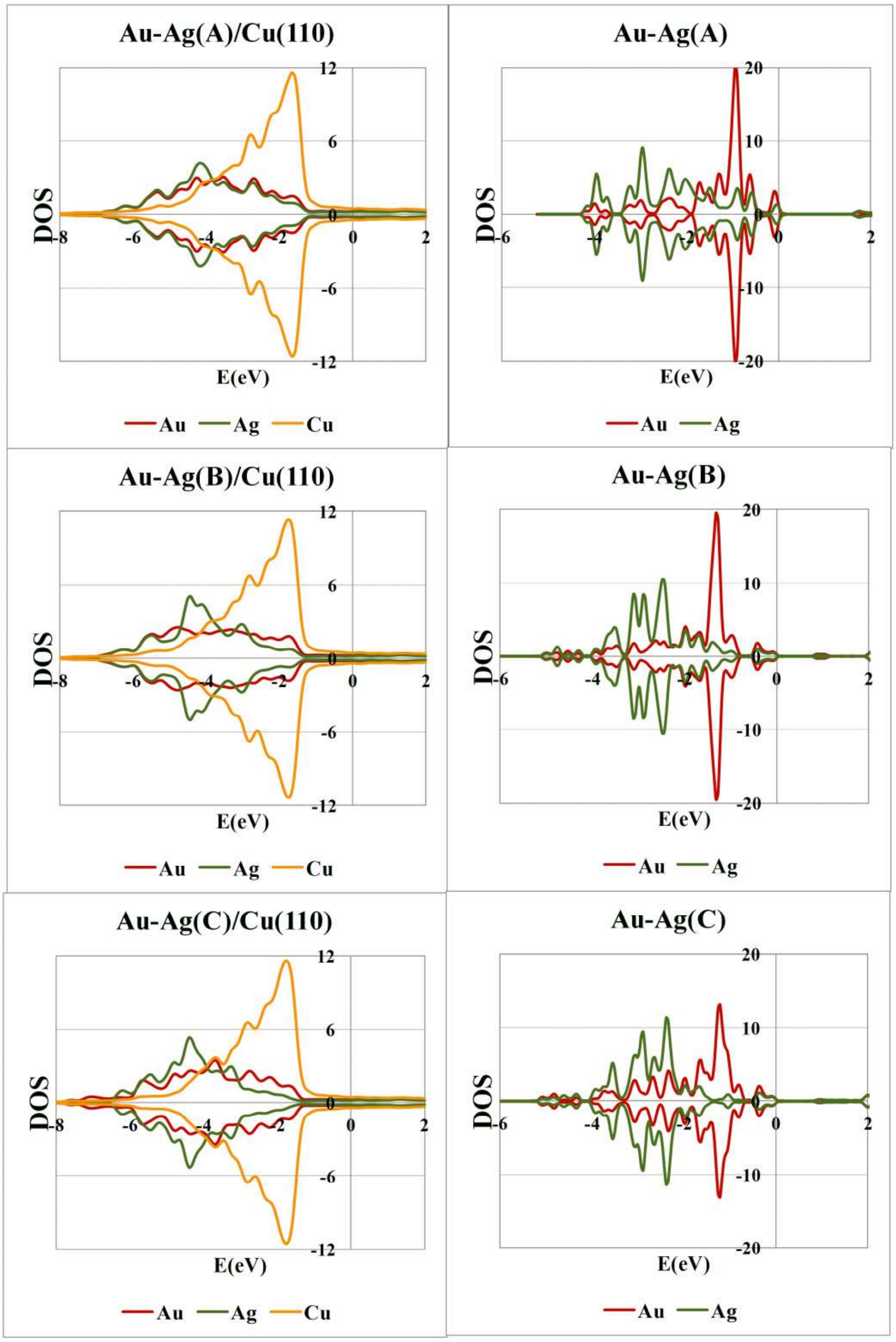

Figure 5.6: PDOS for different configuration of Au-Ag chains on Cu (110) substrate (left panel) and for corresponding free-standing chains of Au-Ag(right panel). The geometries of structures are shown in Fig. 5.2.

This again confirms the stronger tendency of alloying of Au-Ag chains in presence of substrate. As is seen from Fig. 5.6, there is very good orbital overlap of Au and Ag atoms for all the three types in case of Au-Ag double chains placed on Cu(110) substrate.

Our computed PDOS for types A, B and C of double zigzag chains of Au-Ag on Cu(110) substrate are plotted in Fig.5.6. On comparing figures 5.4 to 5.6, we find that the most stable alloyed double zigzag chain structure on Cu(110) substrate appears for the case of Au-Ag. From PDOS and binding energy data it is seen that Au-Ag double zigzag chain structure is stable compared to the single chains of Au-Ag. This is attributed to stronger tendency of alloying of Au and Ag atoms in presence of substrate. It is found that the magnetic moment for both single chain and double chains on the substrate are zero. Unlike the case of single chains on the substrate, where E_{C-C} is lower than E_{C-S} , one can expect a nonzero magnetic moment for double chin structure on substrate. Because, in the case of double chains on Cu(110) substrate, chain atom interaction energy, E_{C-C} is higher than Chain-Substrate interaction energy, E_{C-S} as seen from Table 5.4. Thinking that the cancellation of magnetic moment is resulted from higher chain-substrate interaction, we expected some magnetic moment for the cases of double chains on Cu(110) substrate. However, we do not observe any magnetic moment for all the three configurations of types A, B and C of the double chains of Au-Pd and Au-Pt.

5.4 Conclusion

To summarize, we studied structure and electronic properties of bimetallic chains of Au-Pd, Au-Pt and Au-Ag on two different substrates of NiAl(110) and Cu(110). It is found that the presence of NiAl and Cu substrates significantly influences the electronic structure of the chains. Atoms of single chains of Au-Pd, Au-Pt and Au-Ag bind more strongly with Ni atoms of NiAl substrate, as compared with Cu atoms in Cu(110). The interaction between chain atoms is stronger than the chain-substrate atoms, when chains are placed on Cu substrate, while it is other way round in case of chains on NiAl substrate. On comparing PDOS and interaction energy of free-standing chains of Au-Ag with that of chains placed on the substrate, we find that presence of substrate induces bond formation between Au and Ag atoms which are otherwise not possible in free standing situation.

Another significant change in the presence of the substrate is shifting of d band away from Fermi energy. To study further the effect of increased chain atom interaction, we placed two chains on Cu(110) substrate in three different combinations, termed as A, B and C. It is found that, Au-Pd and Au-Pt bimetallic chains stabilize in double zigzag topology, when placed on Cu(110) substrate. While Au-Ag chains exhibit ladder topology on Cu(110) substrate. The comparison of computed binding energy of three structures, we find that A- type atoms have higher binding energy, as compared to B and C types, when placed on the substrate. Our calculations also show that the magnetic moment of the chain atoms vanish in presence of the substrate. Our plots of interaction energy and PDOS suggest that the magnetic moment is cancelled out due to two reasons: (i) stronger interaction of Pd (Pt) atoms with that of the substrate, and (ii) shifting of orbital away from Fermi energy.