We have investigated the physical properties of gold, nickel nanowires using \textit{ab initio} density functional methods. The total energy minimization and electronic band structure calculations were performed using Vienna \textit{ab initio} simulation package (VASP). The two dimensional, infinite length gold nanowires with 1 – 5 rows of atoms were modeled for different possible structures. It was observed that, parallelogram nanowires are energetically more stable than rectangular shaped nanowires. The stability of parallelogram nanowires can be attributed to the delocalization of $5d$ electrons. The ballistic transport in these nanowires was studied by using Landauer-Büttiker’s formalism. The conductance in gold nanowires shows significant dependence on the structure of the nanowire. Increasing the number of rows of atoms in (100) direction subsequently increases the number of quantized channels for conductance. However, (111) oriented gold nanowires show less number of channels for conduction than the number of atomic rows. In single row nanowire, the conductance is due to $6s$ electron. However, $5d$ electrons contribute in the conductance as the number of rows are increased.

In similarity with gold nanowires, nickel nanowires also show parallelogram motif as the most stable in comparison with the rectangular. Our investigations show that, magnetization in parallelogram shaped nickel nanowires decreases as the number of rows is increased. However, in rectangular nanowires, the magnetic moment initially decreases upto 3 rows of atoms, and then increases. Based on the Stoner’s criterion, $(I * n_{E_f}^0 > 1$, where, $I$ is the exchange integral and $n_{E_f}^0$ denotes number of states at the Fermi energy in nonmagnetic ground state), we observed that, all nickel nanowires with 1 – 6 rows of atoms are ferromagnetic. However, (111) monolayer shows paramagnetic solution indicating possible magnetic transition when the number of rows converge to the film limit. However, no such transition was observed for (100) oriented structures. The nanowires show significant magnetic anisotropy due to spin orbit coupling. It was observed that, the easy axis of magnetization in all nanowires is along the wire axis, except for 3 layered rectangular nanowire. We report this structure to be “magic structure” due to its magnetic anomaly of a smaller magnetic moment, in comparison with the rest of the higher row rectangular structures. The rectangular nanowires show enhanced conductance than that of parallelogram nanowires. The charge carriers for spin up conductance channels in nickel nanowires are mainly of $s$ type, however, spin down channels are mainly of $d$ type with minor $s$ orbital character. The conductance in nickel is affected by spin orbit coupling and shows anistropy with the change in magnetization direction. Nickel nanowires show change in the conductance when the magnetization changes with respect to the current direction. We computed ballistic anisotropic magnetoresistance (BAMR) for nickel nanowires, and observed that, the number of conductance channels are enhanced when the magnetization is perpendicular to the current direction. This observation is reversed for three row parallelogram nanowire, where the conductance channels are enhanced for magnetization parallel to...
current direction.

In addition to pure gold and nickel nanowires, we have also investigated the structural stability of bimetallic Au/Ni nanowires upto 2 rows of atoms, with different concentrations. Our results reveal that, the stability of the bimetallic nanowire is increased with an increase in nickel concentration. Addition of nickel atom in the nanowire enhances the total magnetic moment of the system. The gold atoms in the vicinity of nickel atoms exhibit small magnetic moment due to induced spin polarization.

We have also investigated the antisymmetric exchange (Dzyaloshinskii-Moriya interaction) properties of infinite length bimetallic zigzag nanowires comprised of 3$d$ – 5$d$ elements ($3d \equiv \text{Co, Fe}; 5d \equiv \text{Ir, Pt, Au}$). The calculations were performed using full potential augmented plane wave method in FLEUR. Using the generalized Bloch theorem, the non-relativistic calculations were carried out to obtain spin spiral ground state in a chemical unit cell. Our results show that all 3$d$ – 5$d$ nanowires show degenerate spin spiral ground state except for Fe-Pt and Co-Pt wires. Inclusion of the spin orbit coupling removes the degeneracy in the non-relativistic spin spiral calculations. Relativistic calculations show that, antisymmetric exchange has a significant contribution to the energy of the spin spiral, of the order of $10^{-30}$ meV. Our results show that, ground state structures of Fe-Ir, Fe-Au and Co-Au have left handed spirals, whereas, Co-Pt and Fe-Pt are right handed spiral stabilized. The Dzyaloshinskii-Moriya interaction was found to be vanishing in the direction perpendicular to the wire direction. We analyzed ab initio results with the minimal tight binding model considering the interaction between $d$ orbitals of magnetic site with the non magnetic site. We observed that the degree of hybridization of $d$ orbital plays an important role in the Dzyaloshinskii-Moriya interaction.