The objective of the thesis is focused to enhance the optical responses of the metal nanoparticles (MNPs) by plasmonic coupling between the MNPs and graphene. These optical responses may lead to enhance the scattering and the extinction efficiencies and thus overall efficiency is also enhanced for the photovoltaic. The analytical as well as numerical modeling has been adopted to analyze plasmonic coupling between the graphene and MNPs, which is highly sensitive to the shape, size, and the surrounding environment of the MNPs and the thickness of graphene mono-layer. These parameters play an important role to tune the localized surface plasmon resonances (LSPRs) that are supported by the MNPs. The performance of the Photovoltaics can be boosted by incorporating the concepts of the LSPRs with graphene mono layer, where graphene is used as spacer, substrate, coating material and surrounding environment.

Initially, the analytical approach has been adopted to study the high scattering efficiency of oblate-shaped silver and gold NPs integrated on graphene/silicon substrate under the Quasi-static approximation. Here, graphene is used as spacer that enhances the light confinement inside Si wafer which gives rise to the enhancement in number of absorbed photons in the desired wavelength (400–700nm) domain. Further, the graphene mono layer (GML) is used as a coating material (shell) for the core@shell nanogeometry within the quasi-static approximation. The core@shell (Ag@GML, Au@GML and Al@GML) spherical (3D) nano-particles provide a broad range of the dual surface plasmon resonance (SPR) tunability lies from 300-1500nm wavelength region in the surrounding environment of the TiO₂. This model can also be used to enhance the efficiency of the photovoltaics.

In the next part of this work, the GML coated Ag/Au/Cu Nano-Needle (1D) and Nano-Disk (2D) geometry has been acknowledged in the two different surrounding
environment of the PCDTBT:PC$_{71}$BM and PTB7:PC$_{71}$BM polymer matrix within the Quasi-static approximation. The plasmonic effect of the MNPs embedded in organic polymer matrix has been analyzed to improve the solar cell performance. Such geometries also show desirable resonance tunability in both symmetric (stands for the higher wavelength limit) and anti-symmetric modes (stands for the lower wavelength limit). The analytical approach to study the plasmonic coupling of any realistic arbitrary shaped large nanoparticle is the major challenge for the researchers and scientific community. Therefore, to solve such problems, numerical techniques has been introduced as the surface or the volume discretization.

In order to examine the optical signatures based on volume discretization of oblate, ortho-oblate, prolate and ortho-prolate shaped Ag NPs, discrete dipole approximation (DDA) technique has been used. In this work graphene is used as the surrounding environment for the asymmetric spheroidal shaped Ag nanoparticles (NPs) on Si wafer. The asymmetric spheroidal shaped Ag nanoparticles (NPs) embedded in a graphene monolayer (GML) demonstrates the enhanced performance of graphene/Si Schottky junction solar cells.

In the last section of the work, scattering efficiency of the graphene coated silver-aluminum (Ag-Al) alloy NPs has been calculated which is maximum for 60nm size of NP and saturated after a threshold size. A small red shift arises in scattering efficiency of Ag-Al alloy than the Ag NP is due to the modified optical constant of Ag-Al alloy. Next, silver-aluminum alloy dimer has been examined in presence of humid ambient using DDA technique. Proposed study is useful to enhance the efficiency of the photovoltaics.

Finally, the finding of the thesis provides a guided strategy that how optical signatures of various shaped MNPs can be efficiently tuned under the influence of graphene. The tunable optical signatures of different material nano-geometries in various environments have been significantly used to enhance the photon absorption inside the thin photovoltaic absorber film. The verdict of the present thesis also lead to the experimentalists for selecting the noble
metal type, size, shape, surrounding environment etc. to use the system for variety of applications in scientific and industrial research fields.