Preface

This thesis is devoted to a range of issues in the domain of nanoscience, aimed to solve with experimental and theoretical ventures. The underlying thread of this work is the optimization of NPs for desired applications through experimental executions, navigated by theoretical predictions.

This thesis addresses two main directions. The first one is the experimental approach, which is aimed to exercise different synthetic routes of NPs under colloidal media. In this course of study, the effect of different experimental conditions such as precursor concentrations, surfactant concentrations, temperature, sonication etc. on the geometric parameters of NPs (i.e. size, shape) has been explored. This endeavor has been found to be a candid way to tune NPs for desired functions. The comprehensive characterizations of the NPs are carried out by advanced instrumentation and techniques. This property study is very essential for synthetic NPs to determine to their significant applications.

The second direction is pursued by the theoretical approach. In this approach the unique features especially the optoelectronic nature of NPs has been explored through studies of electronic structure. The theoretical studies are carried out by computational executions of Quantum mechanical approach like Density functional theory (DFT) and Classical Mechanical approach such as Discrete Dipole Approximation (DDA). Finally the attempted correlation between the outcomes of experimental and theoretical studies is found to construct a new route to accomplish the entire goal.