PREFACE

Recent years have witnessed evolution of multifunctional materials to meet the urge of rapidly evolving technological world. To design such materials, optical properties are one of the important characteristics to delve into. Knowledge of the quantum chemical origin of different kind of optical properties in molecules are extremely important for tuning smart materials with desired functionality. We have put our effort to systematically increase the nonlinear optical (NLO) response in molecular systems, which can effectively guide the synthesis of molecules for use in three dimensional memory storage, optical limiting, optical switching etc. In our study, inclusion of zwitterionic substituents has been found to have significant effect on NLO response of molecules, where the push and pull of charges tremendously increase the first hyperpolarizability values. In continuation of our effort to design multifunctional material, coinciding useful magnetic and optical response in the same system seemed to be an interesting idea. There have been reports where organic molecules with both the magnetic and NLO response achieve multifunctionality and this feature is used in the field of biomedicine. From the urge of designing such molecules, we have proposed diradical systems with stable ferromagnetic ground state and reasonable two-photon absorption cross section. Simultaneous presence of these two features makes the systems a promising candidate for magnetic resonance imaging contrast agent and photo sensitizer. Our next work is based on the design of luminescent materials, which have become an indispensable part of our life. In order to construct luminescent devices, specific emitting materials are required amongst which blue emitting materials are rarest for high energy electron transition. This fact motivates us to find out the electronic structural criteria for blue emission, and thus we find appropriate choice of ligands around a 3d transition element can really lead to the electronic transition in blue wavelength region. Such luminescent materials based on 3d transition metals surmount the difficulty of luminescence quenching commonly found in heavy metal-based systems. We also explore the effect of weak interactions like H-bonding on fluorescence. Our study divulges that the H-bonding stabilizes the excited electronic state more compared to the ground state resulting red shift.