PREFACE

The design of smart multifunctional material is essential for the rapidly developing technological world. Magnetic and transport properties are important characteristics to delve into. Since the magnetic status depends on the interaction between magnetic centers, it requires the mechanism of such interaction followed by quantification. On the other hand, transport property depends on how the system is connected to electrodes and the nature of the electrodes. To start with, a crisp discussion about the categories of magnetic materials and the transport property of different spin polarized molecular systems are made in first chapter. Theoretical constructs for the quantification of magnetic and transport properties are discussed in second chapter. It is well known that the extended π-conjugated systems have interesting applications as memory devices, conducting nanowires etc. The transport property of conjugated molecular wires of different length is studied in third chapter to show the effect of length on the electrical transport properties. In this context the magnetic and transport properties of these molecular wires substituted by two radical centers at two different positions are also studied. The fourth chapter deals with the magnetic property of diradicals based on allene and chiral cumulene couplers which contain *sp*-hybridized carbon atoms. Generally, the magnetic exchange coupling constant value decreases with the increase in distance between radical centers in conjugated systems. However, in this chapter we explored that the diradicals based on allene and cumulene coupler have opposite behavior compared to conjugated systems. It is found that spin density distribution within allene and cumulene systems and HOMO-LUMO energy gap has intimate correlation with magnetic property in such systems. These designed systems are ferromagnetic, chiral as well as organic and they may be used as molecular building blocks for organic chiral magnetic solids in future. In the fifth chapter we extend our study towards the magnetic and transport properties of diradicals attached by a range of conjugated coupler and chiral as well as achiral cumulene couplers (which are planar) focusing on the unusual π-interaction properties within the couplers. Transport calculations represent that diradicals based on even cumulene couplers act as better conductor than odd cumulenes couplers (with the increase in chain length of coupler). In the sixth chapter a potential effect of heteroatom substitution within the allene and cumulene couplers in mediating the exchange interaction between the two radical centers is investigated. Several research works show that the presence of heteroatom in the exchange pathway significantly influences magnetic exchange coupling. Interestingly, in heterocumulene based diradicals, tuning of magnetic exchange coupling constant value from antiferromagnetic to ferromagnetic state is observed from *Z*- to *E*- isomer and a unique type of spin delocalization is observed in these systems. In the last chapter, the essence and significance of previous chapters are surmised.