# PREFACE

The phrase "Small Is Beautiful" by a famous economist Leopold Kohr is gradually becoming the keynote to the present scientific community because of the realization of the nanotechnology. Now we live in such a world, where single molecule is going to be applicable in technology. Not only the single molecule device, but also the incorporation of multiple functionalities within that device has been the burning topic of interest for the material scientists. To outline an economic strategy for synthesizing such a molecule or molecular assemblies, *a priori* rational design of the systems based on quantum chemical investigation can be of paramount importance. Thus, in the present work, first we put our effort in explaining the origin of magnetic and conductive properties in different systems. The understanding of the association of quantum chemical nature of the molecular systems with their properties enables us to rationally design molecules with desired degree of magnetic and conductive properties. In designing such systems, we put our focus on the molecules with unpaired spins because the presence of spins is a prerequisite for a system to be magnetic and an optimum candidate for use in spintronics. Modern technology requires a device with unpaired spins and spin transport property. Systems with more than one unpaired electrons have magnetic property which is important in the nanotechnology. Therefore, this work provides the opportunity to be acquainted with the interior of molecular systems and correlate this quantum chemical nature with magnetic and transport property of molecules.