PREFACE

Wiberg once referred aromaticity as a “large fuzzy ball” due to the difficulty in defining the concept precisely. Although aromaticity is popularly considered to be an important concept primarily for organic compounds, but it has been extended to compounds containing transition-metal atoms. Recent findings of aromaticity and antiaromaticity in all-metal clusters have enthused further research in alkaline earth metal clusters referring to their chemical bonding, structures and stability. In this thesis we used the σ-aromatic alkaline earth metal clusters and their alkali metal complexed salts to extended the concept of aromaticity. Motivated by the transformation of σ-aromaticity in free cyclo-$[Mg_3]^{2-}$ to π-aromaticity in the alkali metal salts, we undertake a detailed investigation of the Mg_3Na_2 firstly, to obtain a set of consistent structural data for the species; secondly, to analyze the electronic structure, electron delocalization properties, and aromaticity of these species; and finally, to discuss the changes in aromaticity and emergence of magnetism as a function of the distance from the alkali metal to the center of the Mg_3 ring.

Single molecular magnets have opened an opportunity for the study of physical phenomena at the interface of the microscopic quantum world and the macroscopic classical systems. The field of molecular magnetism has expanded with the discovery of magnetic quantum tunneling in Mn_{12}-acetate molecules. The cornerstone for the rise of present day interest in molecular magnetism owes to the creativity of molecular chemists for designing high and low spin clusters and single chain magnets. There is the vibrant ongoing work on some hole burning phenomenon like molecular spintronics, quantum tunnelling of magnetisation, spin Hall effect etc. The magnetic behaviour in molecules and solids are primarily controlled by exchange interaction. Various microscopic electronic Hamiltonians, spin Hamiltonians have been introduced to solve quantum many body problems and compute magnetic exchange coupling constant. Magnetic anisotropy is responsible for intrinsic ‘easy’ and ‘hard’ directions of the magnetization in some ferromagnetic materials. This magnetic anisotropy is, from both a technological and fundamental viewpoint one of the most important properties of magnetic materials. Owing to the perspective of both fundamental sciences and applications new materials are currently being prepared, named multifunctional molecular materials, which involve interplay or synergy between multiple physical properties like aromaticity and magnetism.