Recent works in our laboratory have shown that novel classes of photo functional metal-containing molecular materials could be assembled through the use of various metal-ligand chromophoric coordination motifs and building blocks. In this presentation, various design and synthetic strategies will be described. A number of these complexes have been shown to display rich optical and luminescence behavior. The optical and luminescence properties have been studied and their origins elucidated. Correlations of the optical and luminescence behavior with the electronic and structural effects of the metal complexes have also been made. These simple discrete metal complexes have also been shown to undergo assembly to give a variety of supramolecular assemblies, nanostructures and morphologies. By understanding the spectroscopic origin and the structure-property relationships, the characteristics of these metal complexes could be fine-tuned for specific applications and functions through rational design and assembly strategies based on the fine interplay of electrostatics and supramolecular non-covalent metal-metal and π-π interactions. These metal-ligand chromophoric complexes may find potential applications and functions as efficient triplet emitters and as luminescence materials for chemosensing, biological assays and molecular imaging.