Chapter 2

Table 2.1. The chemicals used in this study along with the manufacturers are listed below.

Table 2.2. List of various zeoliteY encapsulated transition metal complexes along with their representation and colour.

Chapter 3

Table 3.1. Elemental data analysis (in % by weight).

Table 3.2. ESR spectral parameter data of Cu$^{2+}$ exchanged zeolite, [Cu(Phen)$_3$]$^{2+}$ and Cu-PhenY.

Table 3.3. Oxidation and reduction peak potential values (in V) for neat and the encapsulated M-PhenY (M = Fe$^{2+}$, Cu$^{2+}$ and Zn$^{2+}$) complexes, $E_{1/2} = (E_{\text{oxd}}+E_{\text{red}})/2$.

Table 3.4. Selected bond distance (in Å) and bond angles (in degree) of the optimized neat complexes, [M(Phen)$_3$]$^{2+}$ and zeolite encapsulated phenanthroline complexes, M-PhenY (M = Fe$^{2+}$, Cu$^{2+}$ and Zn$^{2+}$).

Table 3.5. Calculated first ionization potential (IP in eV), electron affinity (EA in eV) energy of HOMO and LUMO (in eV), hardness ($\eta$, in ev), chemical potential ($\mu$, in eV), electrophilicity index ($\omega$ in eV) and global softness ($S$, in eV) of the neat and encapsulated complexes. The values in the parenthesis are obtained using finite difference approximation.

Table 3.6. Calculated first ionization energy (IP) and electron affinity (EA), HOMO and LUMO energies (in eV), hardness ($\eta$, in ev), chemical potential ($\mu$, in eV), electrophilicity index ($\omega$ in eV) and global softness ($S$, in eV) of the encapsulated charged complexes. The values in parenthesis are obtained from finite difference approximation.

Table 3.7. Fukui functions (FFs, $f^+_K$ and $f^-_K$) for the selected atoms of neat [M(Phen)$_3$-Y]$^{2+}$ complexes (M = Fe, Cu and Zn). The values for Cu-complex are those obtained by spin unrestricted calculation.
Table 3.8. Fukui functions (FFs, \( f_k^+ \) and \( f_k^- \)) for the selected atoms of neat [M(Phen)\(_3\)]\(^{2+}\) and M-PhenY complexes (M = Fe, Cu and Zn). The values given in parenthesis are obtained by spin unrestricted calculation.

Table 3.9. Selected energies, oscillator strengths, and expansion coefficients for vertical transitions in [M(Phen)\(_3\)]\(^{2+}\) (M = Fe, Cu and Zn) calculated using a TDDFT approach.

**Chapter 4**

Table 4.1. Binding Energy (eV) for neat and the encapsulated complexes.

Table 4.2. Selected bond distance (in Å) and bond angles (in degree) of the optimized neat complexes, [M(Pic)\(_2\)] and zeolite encapsulated picolinato complexes, [M(Pic)\(_2\)]Y (M = Co, Ni and Cu).

Table 4.3. Calculated energy of HOMO and LUMO (in eV), hardness (\( \eta \), in eV), chemical and global softness (S, in eV).

Table 4.4. Fukui function values for both neat and encapsulated complexes. M= Co, Ni and Cu in respective complexes.

Table 4.5. Oxidation of Phenol by metal chlorides, metal exchanged zeolites, neat and encapsulated picolinato complexes under microwave irradiation in presence of H\(_2\)O\(_2\).

**Chapter 5**

Table 5.1. Elemental analyses for pure NaY, iron exchanged zeolites and zeolite encapsulated complexes.

Table 5.2. FTIR spectral data (in cm\(^{-1}\)) for the neat and the encapsulated Fe-Schiff base complexes.

Table 5.3. UV-vis/DRS spectral data (\( \lambda_{\text{max}} \) in nm) for the uncomplexed ligands, neat and the encapsulated Fe-Schiff base complexes.

Table 5.4. Type of zeolites, Sanderson’s electronegativity and Sanderson’s partial negative charge density on the framework oxygen (-\( \delta_0 \))^a

Table 5.5. EPR analysis of the neat and the encapsulated iron complexes.

Table 5.6. Oxidation and reduction peak potential values (in V) for neat and the encapsulated Fe-Schiff base complexes.

Table 5.7. Selected bond length (in Å) and bond angles (in degree) of the optimized neat and encapsulated Fe-Schiff base complexes.
Table 5.8. Calculated energies of HOMO and LUMO levels (in eV), global hardness ($\eta$, in eV) and softness ($S$, in eV).

Table 5.9. Hirshfeld population analysis of Fukui functions for the neat and the encapsulated complexes.

Table 5.10. Oxidative coupling of 2-naphthol in toluene at 60 °C.

Chapter 6

Table 6.1. Oxidation and Reduction peak potential values (in V) for neat and encapsulated complexes.

Table 6.2. UV-vis/DRS spectral data ($\lambda_{\text{max}}$ in nm) for the uncomplexed ligands, neat and the encapsulated Cu-Schiff base complexes.

Table 6.3. Selected bond length (in Å) and bond angles (in degree) of the optimized neat and encapsulated Cu-Schiff base complexes.

Table 6.4. Calculated energies of HOMO and LUMO levels (in eV), chemical potential ($\mu$, in eV), global hardness ($\eta$, in eV), electrophilicity index ($\omega$, in eV) and softness ($S$, in eV). The values given in parenthesis are those obtained by using IP and EA values.

Table 6.5. Hirshfeld population analysis of Fukui functions for the neat and the encapsulated complexes.

Table 6.6. Henry reaction of $p$-nitro benzaldehyde under various solvent reaction conditions.

Table 6.7. Effect of temperature on the Henry reaction of 4-nitro-benzaldehyde.

Table 6.8. Results of the Henry reaction in presence of various catalysts. The values given in the parenthesis are time (in h) required for completion of the reaction. The (% ee) are calculated from HPLC analysis.