## List of Figures

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>Page no.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Global grand challenges</td>
<td>2</td>
</tr>
<tr>
<td>1.2</td>
<td>World energy consumption (a) by sector and (b) by population</td>
<td>3</td>
</tr>
<tr>
<td>1.3</td>
<td>Total world energy consumption</td>
<td>4</td>
</tr>
<tr>
<td>1.4</td>
<td>Health effects of air pollution</td>
<td>5</td>
</tr>
<tr>
<td>1.5</td>
<td>Biomass to bioenergy</td>
<td>6</td>
</tr>
<tr>
<td>1.6</td>
<td>Methods to convert biomass into various products</td>
<td>7</td>
</tr>
<tr>
<td>1.7</td>
<td>Wind energy to electricity</td>
<td>7</td>
</tr>
<tr>
<td>1.8</td>
<td>Hydro power</td>
<td>8</td>
</tr>
<tr>
<td>1.9</td>
<td>Geothermal Energy</td>
<td>9</td>
</tr>
<tr>
<td>1.10</td>
<td>Comparison of solar energy with other energy forms</td>
<td>10</td>
</tr>
<tr>
<td>1.11</td>
<td>A p-n junction and depletion region</td>
<td>12</td>
</tr>
<tr>
<td>1.12</td>
<td>Different types and generations of solar cell</td>
<td>13</td>
</tr>
<tr>
<td>1.13</td>
<td>Classic silicon solar cells- (a) Monocrystalline solar cell (b) polycrystalline solar cell</td>
<td>13</td>
</tr>
<tr>
<td>1.14</td>
<td>Thin film solar cell</td>
<td>14</td>
</tr>
<tr>
<td>1.15</td>
<td>Organic solar cell</td>
<td>15</td>
</tr>
<tr>
<td>1.16</td>
<td>DSSC device architecture</td>
<td>18</td>
</tr>
<tr>
<td>1.17</td>
<td>Evolution of different types of sensitizers</td>
<td>19</td>
</tr>
<tr>
<td>1.18</td>
<td>Commercially available ruthenium dyes</td>
<td>20</td>
</tr>
<tr>
<td>1.19</td>
<td>Structure of organic dyes exhibiting high efficiency</td>
<td>21</td>
</tr>
<tr>
<td>1.20</td>
<td>Working principle of DSSC</td>
<td>26</td>
</tr>
<tr>
<td>1.21</td>
<td>Kinetics involved in each step of DSSC</td>
<td>28</td>
</tr>
<tr>
<td>1.22</td>
<td>IV parameters of solar cell</td>
<td>29</td>
</tr>
<tr>
<td>1.23</td>
<td>The Ragone plot</td>
<td>33</td>
</tr>
<tr>
<td>1.24</td>
<td>Double layer capacitors</td>
<td>34</td>
</tr>
<tr>
<td>1.25</td>
<td>Classification of supercapacitors</td>
<td>35</td>
</tr>
<tr>
<td>1.26</td>
<td>Mechanisms for (a) double layer, (b) pseudocapacitor and (c) Li-battery</td>
<td>36</td>
</tr>
<tr>
<td>1.27</td>
<td>Potential energy of an electron as a function of distance x</td>
<td>42</td>
</tr>
</tbody>
</table>
Figure 1.28: Variety of architectures of polymers ................................................. 46
Figure 1.29: Applications of polymers .................................................................. 46
Figure 1.30: Polymers for various energy applications ......................................... 47
Figure 1.31: Few representative examples of conjugated polymers ................. 49
Figure 1.32: Conjugated polymers: perspective ................................................... 50
Figure 1.33: Representation of the band gap modulation with the increasing number of repeating units .......................................................... 51
Figure 1.34: Basic structure of PPV ................................................................. 53
Figure 1.35: Gilch polymerization approach ....................................................... 53
Figure 1.36: Chemical vapor deposition for synthesis of PPV ......................... 54
Figure 1.37: Olefin metathesis polymerizations for synthesis of PPV .............. 55
Figure 1.38: Wittig type polymerization methods for synthesis of PPV ............ 55
Figure 1.39: Palladium catalyzed reactions for synthesis of PPV .................... 56
Figure 1.40: Overview of the use of polymers in energy storage systems ....... 58
Figure 2.1: DSSC device fabrication ................................................................. 73
Figure 2.2: Schematic representation of NMR spectroscopy system .................. 75
Figure 2.3: Schematic description of UV-Vis setup .......................................... 76
Figure 2.4: Photoluminescence Spectroscopy- schematic representation ......... 78
Figure 2.5: Schematic diagram of FTIR system ............................................. 79
Figure 2.6: Raman spectroscopy diagram .......................................................... 80
Figure 2.7: Mechanism of X-ray diffraction ....................................................... 81
Figure 2.8: Schematic illustration of XPS .......................................................... 83
Figure 2.9: SEM instrument and mechanism ..................................................... 84
Figure 2.10: TEM setup ..................................................................................... 86
Figure 2.11: Schematic representation of AFM .................................................. 87
Figure 2.12: TGA diagramatic representation .................................................... 88
Figure 2.13: GPC setup ..................................................................................... 89
Figure 2.14: BET analysis instrument ............................................................... 90
Figure 2.15: A typical cyclic votammogram ...................................................... 92
Figure 2.16: CV potential waveform ................................................................. 92
Figure 2.17: (a) Schematic representation of solar simulator, (b) Instrument photograph of solar simulator at CSIR-National Chemical Laboratory .................................................................................. 94
Figure 2.18: (a) Configuration of planer diode system, (b) Field emission
setup........................................................................................................... 95

Figure 3.1: $^1$H NMR spectra of PPV A, PPV CHO and PPV acid.............. 104
Figure 3.2: UV-Vis spectra of PPV A and PPV acid....................................... 105
Figure 3.3: DRS spectra of PPV A and PPV acid............................................. 106
Figure 3.4: Photoluminescence spectra of (a) PPV A and (b) PPV acid........ 106
Figure 3.5: FTIR spectra of PPV A, PPV CHO and PPV acid (inset showing expanded portion of carbonyl region)....................................................... 107
Figure 3.6: Band alignment of PPV A and PPV acid with TiO$_2$.................... 108
Figure 3.7: J-V characterization for (a) PPV A and PPV acid, (b) comparison of J-V curves for PPV A, PPV CHO and PPV acid........................................ 109
Figure 3.8: (Top) TiO$_2$ films sensitized with PPV A, PPV CHO and PPV acid by dipping in their chloroform solutions (Below)................................. 110
Figure 3.9: IPCE measurements of PPV A and PPV acid dye loaded TiO$_2$ films ................................................................................................. 111
Figure 3.10: Force-distance curves taken at four different locations on bare and PPV acid dye-loaded TiO$_2$ surface .......................................................... 112
Figure 3.11: STM Spectra taken on bare TiO$_2$ and PPV acid dye loaded TiO$_2$. 113
Figure 3.12: STM Topography and line scan on bare TiO$_2$ and PPV acid dye loaded TiO$_2$ ...................................................................................... 114
Figure 3.13: TG curves of PPV A and PPV acid .............................................. 114
Figure 3.14: Solar conversion efficiency with respect to cell processing temperature ........................................................................................................ 115
Figure 4.1: Representation and mechanism of click reaction................................ 123
Figure 4.2: (a) Illustration of the strategic design of the precursor structure, (b) molecular representation of P3K in 3D (Element ID: grey small ball C, grey big ball K, white ball H, blue ball N and red ball O).............. 129
Figure 4.3: FTIR spectra of polymers P1, P2 and P3 ........................................ 131
Figure 4.4: (a) $^1$H NMR spectrum of P1 [poly(4-chloromethylstyrene)], (b) $^1$H NMR spectrum of P2 [poly(4-azidomethylstyrene)] and (c) $^1$H NMR spectrum of P3 [carboxylic acid functionalized triazole ring-containing polystyrene] ..................................................................................... 133
Figure 4.5: (a) Powder XRD pattern of P3KC, (b) Raman spectrum of P3KC . 134
Figure 4.6: Raman Spectra of (a) P1C and (c) P3C, Powder X-ray diffraction pattern of (b) P1C and (d) P3C ................................................................. 134
Figure 4.7: (a) and (b) FESEM images of P3KC at different scales................. 135
Figure 4.8: (a), (b) and (c): HRTEM images of P3KC at different scales, (d) lattice fringes pattern obtained for P3KC .................................................. 136
Figure 4.9: XPS of P3KC: (a) C1s, (b) O 1s, (c) N1s.................................................. 137
Figure 4.10: (a): Pore size distribution of P3KC acquired from DFT calculations, (inset- cumulative pore volume) (b) N2 adsorption-desorption isotherm for P3KC. .............................................................. 138
Figure 4.11: (a) Cyclic voltammogram (CV) of P3KC in 1M H2SO4 as electrolyte at the scan rate of 100 mV s⁻¹, (b) Galvanostatic charging-discharging data for P3KC at the current density of 1 Ag⁻¹ ................................................................. 141
Figure 4.12: (a) CV of P3KC in TEABF₄ as electrolyte at different scan rates in the potential range of 0-2.7 V, (b) Galvanostatic charging-discharging data for P3KC at the various current densities. ............ 141
Figure 4.13: (a) Specific capacitance measured from charging-discharging at different current densities, (b) Ragone plot .............................................. 142
Figure 4.14: Cyclic stability data of organic EDLC measurements for P3KC case in the coin-cell assembly.......................................................... 143
Figure 4.15: Comparison of impedance measurements (Nyquist plot) between coin cell and Swagelok cell assembly for P3KC ......................... 144
Figure 4.16: (a) Typical charging-discharging curves for Li/P3KC half-cell, (b) half cell cyclic stability from 3 V to 4.6 V at the current density of 100 mA g⁻¹, (c) Galvanostatic charging-discharging curves for P3KC/ Li₄Ti₅O₁₂ Li-HEC at different current densities between 1V to 3V, (d) Ragone plot of P3KC/ Li₄Ti₅O₁₂ and commercial AC/ Li₄Ti₅O₁₂, (e) Cyclic stability of P3KC/ Li₄Ti₅O₁₂ at the current density of 2 A g⁻¹ ................................................................. 145
Figure 5.1: Polymer film preparation ................................................................. 158
Figure 5.2: ¹H spectrum of 5,10-dioctyl-5,10-dihydrophenazine ....................... 162
Figure 5.3: ¹H NMR spectrum of 5,10-dioctyl-5,10-dihydrophenazine-2,7-dicarbaldehyde recorded in CDCl₃ ......................................................... 162
Figure 5.4: ¹H NMR spectrum of tetraethyl (2,5-bis((2-ethylhexyl) oxy)-1,4 phenylene) bis(methylene)bis(phosphonate) recorded in CDCl₃ .... 163
Figure 5.5: ¹³C spectrum of 5,10-dioctyl-5,10-dihydrophenazine recorded in
Benzene d₆ ................................................................. 164

Figure 5.6: $^{13}$C NMR spectrum of 5,10-dioctyl-5,10-dihydrophenazine-2,7-dicarbaldehyde recorded in Benzene d₆................................. 164

Figure 5.7: MALDI spectrum of monomer (3) 5,10-dioctyl-5,10-dihydrophenazine-2,7-dicarbaldehyde................................. 165

Figure 5.8: MALDI spectrum of monomer (6) - tetraethyl ((2,5-bis((2-ethylhexyl) oxy)-1,4 phenylene) bis(methylene))bis(phosphonate)........ 166

Figure 5.9: $^1$H NMR spectrum polymer PHN-PPV................................. 167

Figure 5.10: (a) UV visible spectrum of the PHN-PPV in chloroform solution, (b) Photoluminescence spectrum of PHN-PPV in chloroform solution. ................................................................. 167

Figure 5.11: Cyclic voltammetry for PHN-PPV at the scan rate of 100 mV/s... 168

Figure 5.12: TG curve of PHN-PPV in the nitrogen atmosphere.................. 169

Figure 5.13: HOMO and LUMO levels of the monomer of PHN-PPV .......... 170

Figure 5.14: (a) Mott-Schottky measurements, (b) AC conductivity measurements ................................................................. 170

Figure 5.15: (a) Emission Current density versus applied electric field (J-E) plot, (b) F-N plot ................................................................. 172

Figure 5.16: Stability of the field emitter over the duration of 6 hrs.............. 173

Figure 5.17: SEM images of the film before (a) and after (b) the FE measurement. ................................................................. 173

Figure 5.18: Field emission images ................................................................. 174

Figure 6.1: Donor-acceptor conjugated polymers for organic solar cells ........ 184

Figure 6.2: PPV derivatives for LED applications .................................................. 185

Figure 6.3: Representative structure of polymer for hole transport material application ........................................................................ 186
### List of Schemes

<table>
<thead>
<tr>
<th>No.</th>
<th>Description</th>
<th>Page no.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Scheme 3.1: Synthesis of <strong>PPV acid</strong></td>
<td>103</td>
</tr>
<tr>
<td></td>
<td>Scheme 4.1: Synthesis of polystyrene derivative-a polymeric precursor (P3K) for porous carbon.</td>
<td>130</td>
</tr>
<tr>
<td></td>
<td>Scheme 5.1: Synthesis of monomers (3) and (6)</td>
<td>160</td>
</tr>
<tr>
<td></td>
<td>Scheme 5.2: Synthesis of <strong>PHN-PPV</strong></td>
<td>160</td>
</tr>
</tbody>
</table>