

## LIST OF TABLES

<b>Table 3.1.</b>	The lattice parameters, bulk modulus and pressure derivative of bulk modulus of GaX compounds in ZB and WZ phases.....	<b>65</b>
<b>Table 3.2.</b>	The electronic bandgaps and bandgap types of GaX compounds in ZB and WZ phases.....	<b>66</b>
<b>Table 3.3.</b>	The acoustic and optic phonon frequencies at high-symmetry points of BZ, the Born effective charges ( $Z^*$ ) and high frequency di-electric constants ( $\epsilon$ ) for ZB GaX compounds.....	<b>72</b>
<b>Table 3.4.</b>	The vibrational frequencies of phonon modes, Born effective charges ( $Z^*$ ) and high frequency di-electric constants ( $\epsilon$ ) of WZ GaX compounds.....	<b>73</b>
<b>Table 3.5.</b>	Calculated hole effective mass ( $m_h^*$ ), deformation potential ( $E_1$ ), elastic constant ( $C_{ii}$ ), hole mobility ( $\mu$ ) and relaxation time ( $\tau$ ) of GaX compounds in ZB and WZ phases.....	<b>77</b>
<b>Table 3.6.</b>	Lattice thermal conductivity ( $\kappa_l$ ) at 300 K for GaX compounds in ZB and WZ phases.....	<b>82</b>
<b>Table 3.7.</b>	The structural and electronic properties of GaX (X=P, As, Sb) nanowires for three different diameters.....	<b>90</b>
<b>Table 3.8.</b>	The structural and electronic parameters of GaP1, GaAs1 and GaSb1 NWs under the effect of uniaxial compressive strain.....	<b>95</b>
<b>Table 4.1.</b>	Computed structural and electronic parameters of GaSb-GaAs and GaSb-GaP HSNWs together with pristine GaP, GaAs and GaSb NWs.....	<b>123</b>
<b>Table 4.2.</b>	Computed solar cell parameters for GaX (X=P, As, Sb) NWs under SQ limit. ....	<b>133</b>
<b>Table 4.3.</b>	Computed solar cell parameters of GaSb-GaAs and GaSb-GaP HSNWs together with their comparison to the pristine core and shell NWs. ...	<b>133</b>
<b>Table 5.1.</b>	Computed structural and electronic parameters of AlX (X=P/As) in bulk, nanowire (NW) and radial (R) and axial (A) heterostructure nanowire (HSNW) configurations.....	<b>146</b>
<b>Table 6.1.</b>	Computed structural parameters of WZ BP in bulk and NW configurations.....	<b>171</b>
<b>Table 6.2.</b>	Electronic band gap ( $E_g$ ), electron effective mass ( $m_e^*$ ) and nature of band gap of Boron Phosphide in bulk and NW geometries.....	<b>171</b>

<b>Table 6.3.</b>	Computed bond lengths and angles of BP NW subjected to hydrogen adsorption at different sites of NW surface.....	<b>176</b>
<b>Table 6.4.</b>	Computed bond lengths and angles of BP NW subjected to oxygen adsorption on different sites of NW surface.....	<b>181</b>
<b>Table 6.5.</b>	Adsorption and Gibbs free energies (in electron-volts) of BP NW under hydrogen and oxygen adsorption for pristine and Al and Ga doped configurations.....	<b>184</b>
<b>Table 6.6.</b>	Computed adsorption energy, Gibbs free energy and distance between the hydrogen atom to NW surface.....	<b>191</b>
<b>Table 6.7.</b>	The computed values of bond-length and distance of adsorbed hydrogen from NW surface.....	<b>191</b>
<b>Table 6.8.</b>	Computed bond angles of pristine and defected GaP NW with corresponding adsorption energy.....	<b>192</b>