LIST OF FIGURES

Figure 1.1.	Energy dependent responses of electronic density of states (DOS) for bulk, 2D and 1D materials. The crystal structures and DOS equations are embedded with respective systems
Figure 1.2.	Profiles of number of publications versus year of publication is presented for (a) DFT, (b) Nanowires (NWs) and (c) Heterostructure Nanowires (HSNWs) (source: Web of Science as on June-2020)
Figure 1.3.	Confinement dependent modulation in electronic properties of gallium phosphide (GaP): from bulk to 1D nanowires with three distinct diameters (atoms in green, orange and yellow represent gallium, phosphorous and hydrogen atoms, respectively)
Figure 1.4.	Three distinct types of heterostructures (type-I, type-II and type-III) formed when semiconductor materials (A and B) with different band edge alignments are merged (yellow and blue bars represent the bandgap magnitude of A and B semiconductor materials, respectively.).
Figure 3.1.	The DFT computed electronic dispersion curves for (a, d) GaP, (b, e)
U	GaAs and (c, f) GaSb in ZB and WZ phases, respectively67
Figure 3.2.	The computed electronic density of states (PDOS) plots as a function of energy for (a, d) GaP, (b, e) GaAs and (c, f) GaSb in ZB and WZ phases, respectively
Figure 3.3.	The DFPT computed phonon dispersion curves (PDCs) and respective phonon density of states (PHDOS) curves for (a, d) GaP, (b, e) GaAs and (c, f) GaSb in ZB and WZ phases, respectively
Figure 3.4.	QHA computed thermodynamic functions (a) Entropy, (b) Specific heat, (c) Vibrational Energy and (d) Internal energy of GaX compounds in ZB phase
Figure 3.5.	QHA computed thermodynamic functions (a) Entropy, (b) Specific heat, (c) Vibrational Energy and (d) Internal energy of GaX compounds in WZ phase
Figure 3.6.	Calculated temperature dependent electronic contributions to the thermoelectric properties of the GaX compounds in ZB phase: (a) Seebeck co-efficient, (b) electrical conductivity, (c) Power factor and (d) electronic contributions to thermal conductivity

- **Figure 3.8.** Computed phonon dependent thermoelectric parameters (a, d) Phonon group velocity, (b, e) Mode Gruneisen parameters and (c, f) Phonon scattering rate for GaX compounds un ZB and WZ phases, respectively.
- **Figure 3.9.** Calculated thermoelectric parameters as a function of temperature (a, b) Thermal conductivity, (c, d) Electronic Figure of Merit and (e, f) Overall Figure of Merit for GaX compounds in ZB and WZ phases, respectively.

- Figure 3.10. Optimized top and side views of hydrogen passivated gallium phosphide nanowires (GaP NWs) with diameters ~ 1 (GaP1), 2 (GaP2) and 3 (GaP3) nm. (Spheres in green, orange and mustered yellow represent atoms of gallium, phosphorous and hydrogen, respectively.)
- **Figure 3.12.** Optimized top and side views of hydrogen passivated gallium antimonide nanowires (GaSb NWs) with diameters ~ 1 (GaSb1), 2 (GaSb2) and 3 (GaSb3) nm. (Spheres in green, pink and mustered yellow represent atoms of gallium, antimony and hydrogen, respectively.......88

Figure 3.19.	Modulation in electronic band structure of GaSb NW subjected to uniaxial compressive strain
Figure 3.20.	Strain dependent electronic edge states (VBM/CBM) of GaP1, GaAs1 and GaSb1 NWs
Figure 3.21.	Diameter dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaP NW98
Figure 3.22.	Diameter dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaAs NW99
Figure 3.23.	Diameter dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaSb NW 100
Figure 3.24.	Strain dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaP NW 101
Figure 3.25.	Strain dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaAs NW 102
Figure 3.26.	Strain dependent modification in the optical properties (a) Real part of di-electric function ε_1 , (b) Imaginary part of di-electric function ε_2 , (c) Extinction co-efficient k(ω), (d) Refractive index η , (e) Loss function L(ω), (f) Reflectivity R(ω) and (g) Absorption co-efficient α of GaSb NW 103
Figure 4.1.	Top and Side views of optimized crystal structures of GaSb-GaAs and GaSb-GaP HSNWs with round (R) and triangular (T) cores, respectively. The atoms in Green, Pink, Purple, Orange and Yellow represent the atoms of Ga, Sb, As, P and H, respectively
Figure 4.2.	Computed electronic band structures of GaSb-GaAs and GaSb-GaP HSNWs with round (R) and triangular (T) cores, respectively 124
Figure 4.3.	Computed partial electronic density of states (PDOS) of GaSb-GaAs (a, b) and GaSb-GaP (c, d) HSNWs with round (R) and triangular (T) cores, respectively 126

Figure 4.4.	Computed electronic band structures of individual core and shell NWs of GaSb-GaAs HSNW with round (upper panel) and triangular (lower panel) cores, respectively
Figure 4.5.	Computed electronic band structures of individual core and shell NWs of GaSb-GaAs HSNW with round (upper panel) and triangular (lower panel) cores, respectively
Figure 4.6.	Schematic representation of band edge alignments (not to the scale) of GaX (P/As/Sb) in bulk and NW forms and for core and shell NWs of corresponding HSNWs with GaSb NW as a shell NW (The schematic diagram on the top represent the crystal structures of the systems under bulk, NW and HSNWs dissected into core and shell structures with corresponding electronic band gaps in eV)
Figure 4.7.	Computed real and imaginary components of complex di-electric function as a function of photon frequency for GaSb-GaAs and GaSb-GaP HSNWs for round (R) and triangular (T) cores, respectively 131
Figure 4.8.	Computed absorption co-efficient of GaSb-GaAs (a, b) and GaSb-GaP (c. d) HSNWs with round (R) and triagular (T) core, respectively. The insets of the graphs represent reflectivity of corresponding system 132
Figure 4.9.	Computed JV curve for GaX (X=P, As, Sb) NWs and GaSb-GaX (X=As, P) HSNWs with comparison to the pristine GaP, GaAs and GaSb NWs.
Figure 5.1.	Optimized crystal structures of aluminium phosphide (AlP) in bulk (a) cubic zincblende (ZB) and (b) hexagonal Wurtzite (WZ), and (c) nanowire (NW) Phases. The spheres in blue, brown and yellow represent the atoms of aluminium, phosphorous and hydrogen, respectively
Figure 5.2.	Optimized crystal structures of aluminium arsenide (AlAs) in bulk (a) cubic zincblende (ZB) and (b) hexagonal Wurtzite (WZ), and (c) nanowire (NW) Phases. The spheres in blue, green and yellow represent the atoms of aluminium, arsenic and hydrogen, respectively147
Figure 5.3.	Electronic dispersion curve for aluminium phosphide (AlP) in cubic zincblende (ZB), hexagonal Wurtzite (WZ) and nanowire (NW) configurations149
Figure 5.4.	Electronic dispersion curve for aluminium arsenide (AlAs) in cubic zincblende (ZB), hexagonal Wurtzite (WZ) and nanowire (NW) configurations 149

Figure 5.5.	Phonon dispersion curve for aluminium phosphide (AlP) and aluminium arsenide (AlAs) in cubic zincblende (ZB) and hexagonal Wurtzite (WZ) phases
Figure 5.6.	Real (ϵ_r) and imaginary (ϵ_i) components of complex di-electric function for aluminium phosphide (AlP) ad aluminium arsenide (AlAs) in cubic zincblende (ZB), hexagonal Wurtzite (WZ) and nanowire (NW) configurations
Figure 5.7.	Absorption co-efficient (α) and joint density of states (JDOS) as a function of photon energy for aluminium phosphide (AlP) and aluminium arsenide (AlAs) in cubic zincblende (ZB), hexagonal Wurtzite (WZ) and nanowire (NW) configurations
Figure 5.8.	Optimized crystal structures of radial heterostructure nanowires (HSNWs) with core/shell geometry (a) AlP/AlAs (R) and (b) AlAs/AlP (R) and, (c) axial HSNW AlP/AlAs (A) with AlP and AlAs NWs stacked on top of each other. The atoms in blue, brown, green and yellow represent respectively the atoms of aluminium, phosphorous, arsenic and hydrogen
Figure 5.9.	Computed electronic band structure for radial (R) heterostructure nanowires (HSNWs) with core/shell geometry AlP/AlAs (R) and AlAs/AlP (R), and, axial HSNW AlP/AlAs (A) with AlP and AlAs NWs stacked on top of one-another
Figure 5.10.	Computed electronic band structures of individual heterolayer core/shell for radial (R) heterostructure nanowires (HSNWs) (a) AlP/AlAs, (b) AlAs/AlP and, (c) AlP/AlAs (A) HSNW with bottom/top stacking of heterolayers 158
Figure 5.11.	Real (ϵ_r) and imaginary (ϵ_i) components of complex di-electric function (a, b), absorption co-efficient α (c) and joint density of states (JDOS) (d) for AlP/AlAs and AlAs/AlP radial (R) heterostructure nanowires (HSNWs) and AlP/AlAs axial (A) HSNW configurations 160
Figure 6.1.	Top and Side views of optimized crystal structure of pristine BP NW (atoms in yellow, red and green represent boron, phosphorous and hydrogen atoms, respectively.)
Figure 6.2.	(a) Electronic Band Structure with corresponding density of states (DOS) and (b) partial electronic density of states (PDOS) of BP NW 172
Figure 6.3.	Top and side views of BP NW doped with aluminium (a, b) and gallium (c, d) respectively (atoms in purple and blue are aluminium and gallium, respectively.)

Figure 6.4.	Top and side views of BP NW with hydrogen adsorbed on two distinct surface sites (a, b) Site-A and (c, d) Site-B175
Figure 6.5.	Top and side views of BP NW subjected to hydrogen adsorption on Site-A (a, b) and Site-B (c, d) respectively
Figure 6.6.	Partial density of states (PDOS) of BP NW in (a) pristine and, H adsorbed on (b) Site-A and (c) Site-B, respectively 178
Figure 6.7.	Top and side views of BP NW before adsorbing oxygen atom on site-A (a, b) and site-B (c, d) respectively 180
Figure 6.8.	Top and side views of BP NW subjected to oxygen adsorption on Site-A (a, b), and, Site-B (c, d) respectively 182
Figure 6.9.	Partial density of states (PDOS) of BP NW in (a) pristine and O adsorbed on (b) Site-A and (c) Site-B, respectively 183
Figure 6.10.	Cross sectional view (upper panel) and side view (lower panel) of Gallium Phosphide nanowire (a) Pristine NW (b) B-substituted NW and (c) N-substituted NW (atoms in purple, yellow, red, green and cyan represent respectively the atoms of gallium, phosphorous, boron, nitrogen and hydrogen)
Figure 6.11.	Computed electronic band structures of a) pristine, b) Boron defected and c) Nitrogen defected GaP NW
Figure 6.12.	Partial electronic density of states of a) pristine, b) Boron defected and c) Nitrogen defected GaP NW
Figure 6.13.	Top and Side views of GaP pristine NW before complete adsorption of hydrogen on (a) Site-A, (b) Site-B and (c) Site-C 189
Figure 6.14.	Top and Side views of pristine GaP NW after adsorption of hydrogen on (a) Site-A, (b) Site-B and (c) Site-C 190
Figure 6.15.	Top and side views of a) pristine, b) Boron defected and c) Nitrogen defected GaP NW after adsorbing hydrogen on NW surface 192
Figure 6.16.	Partial density of states (PDOS) of a) pristine, b) Boron defected and c) Nitrogen defected GaP NW after adsorbing hydrogen on NW surface
Figure 7.1.	The computed electronic band structures of GaP NWs under the effect of external strain and size modulation
Figure 7.2.	Schematic representation of band edge alignments (not to the scale) of GaX (P, As, Sb) in bulk and NW forms and for core and shell NWs of corresponding HSNWs with GaSb NW as a shell NW (The schematic

	diagram on the top represent the crystal structures of the systems under
	bulk, NW and HSNWs dissected into core and shell structures with
	corresponding electronic band gaps in eV)203
Figure 7.3.	Optimized crystal structures of AlAs/AlP (R), AlP/AlAs (R) and AlP/AlAs (A) HSNWs with their corresponding electronic dispression
	curves