Energetics, Structural and Optoelectronic Properties of III-V Semiconductor Heterostructure Nanowires

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Name of the Student	:	**Trupti K. Gajaria**
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Name of the Supervisor	:	**Prof. Prafulla Kumar Jha** **Department of Physics, Faculty of Science** **The Maharaja Sayajirao University of Baroda, Vaodara-390002, Gujarat, India.**
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Place of Work	:	**Department of Physics, Faculty of Science, The Maharaja Sayajirao University of Baroda, Vadodara-390002, Gujarat, India.**

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Introduction

Thanks to the high-throughput research and development made in the field of energy applications in the past few decades, it has provided the world with novel materials possessing unique properties. Amongst the latest cutting-edge fields, the three major contributing fields are the photo-voltaics, opto-electronics and thermoelectrics. Interestingly, the materials from group III-V, like GaN, GaAs, GaP, BN, BP, AlN, InAs, InSb, etc., that have been studied have found applications in all the three fields. Further refinement in the properties of these materials can be achieved by means of chemical doping or by applying external pressure/strain or by imposing quantum confinement. The term quantum confinement relates with the word 'nano' (measuring one billionth part of a unit) that is derived from the Greek word '***nanus***' meaning *dwarf*, has been declared as a standard prefix by CGPM committee in 1960. A mysterious modulation in the material properties was observed as a result of a just reduction in its dimension/s, this was given the name quantum confinement effect. This depends on the number of reduced/confined dimensions; i.e. zero-, one- and two- dimensional nanostructures have respectively three, two and one confined dimension/s. Among the three distinct nanostructures, the two-dimensionally confined one-dimensional (1D) nanostructures like nanotubes, nanoribbons and nanowires have grabbed the greatest attention owing to their versatile properties like strong quantum confinement[1], carrier trapping[2,3] and moderate electronic bandgaps[4,5]. Plenty of research articles explaining the growth mechanism[6], phase engineering[7,8] and heterostructuring[9,10] of the NWs emphasize the significance of these one-dimensional (1D) systems owing to their versatile nature and

multiple applicability. Further, these 1D systems, especially when constructed by combining the group III and V elements, yield tremendously unexpected results[11]. One can also find vast documentation on the dramatic behaviour of the III-V nanowires when subjected to heterostructuring[12,13]; especially, as through in this method, the spatial electronic states, which are already modified through imposition of two-dimensional confinement, are still subjected to finer modulation to achieve desired transport through the system qualitatively and quantitatively[14–17]. As it has been usually observed, introducing heterostructured geometry causes lattice mismatch between the host/core material and the masking/shell material due to difference in their lattices under pristine conditions. This could be one of the factors responsible for trapping/separating the charge carriers or for elongating the carrier lifetimes/recombination rates;[18,19,20] this further helps to understand the transport mechanism taking place at the hetero-interface. For obtaining desired properties with feasible stability, it is expected that the lattice mismatch between the host/reference and masking/stacking material should be minimum or within an acceptable range. More the lattice mismatch, more the strain generated in the system. Although in the case of one-dimensional heterostructure nanowires, the generated strain gets released in radial directions and stability is achievable with unique interface properties. Literature survey on III-V HSNWs for the past few decades reveals successful synthesis of radial and axial HSNWs by employing VLS method which not only felicitates the growth of HSNWs with distinct lattice constants of shell and core materials but also possesses large lattice mismatch with the substrate material,[21–24] the prime reason being the release of strain through free nanowire

surface via radial direction. One of the studies on GaAsP/GaP core-shell NW by Himwas et al.[25,26] shows unintentional occurrence of core-shell geometry on deviating the As and P content in GaAsP NW. Further, it is observed that without passivation these NWs do not show markable luminescence properties; however, on passivating the NW with GaP shell it induces extra peak in PL spectra, confirming optical transition. Zhang et al.[27,28] have suggested strong carrier confinement owing to large differences in the bandgaps of core and shell nanowires on combining III-V HSNWs with V material shell. The resultant downward surface band bending causes enhancement in the carrier injection efficiency of the system. The present thesis covers a systematic investigation on the structural, electronic, optical and vibrational properties of selected III-V NWs utilizing well-established quantum mechanical tool density functional theory (DFT).[29] To get deep insight into the underlying mechanism of carrier dynamics within the heterostructured configuration, and to establish a relation between the properties of the system under bulk, NW and HSNW geometries, a comparative assessment of evaluated properties is carried out.

Objectives

The foremost objective of the present research work is to study the effects of two-dimensional quantum confinement on the structural, electronic, optical and transport properties of the systems constructed by combining the selected elements from group III with group V. The motivation behind selecting III-V compounds is their unique properties that can further be tuned or modulated according to the applications like

photovoltaic solar cells, high-frequency field effect transistors (FETs), opto-electronic devices or thermoelectric devices. Imposing two-dimensional confinement on these materials to form one-dimensional nanowires is a unique approach for tailoring the material properties like enhancement in electro-optic transport and carrier effective masses. Further enrichment in the transport properties and in overall efficiency can be achieved by means of confining the charge carriers within separate regions of the nanowire via construction of heterostructure by a combination of two or more layers/shells of distinct materials.

The specific objectives of the present study are as under:

1. To optimize the selected III-V compounds with their polytypic bulk phases and compute their electronic, optical and thermoelectric properties.
2. To construct two-dimensional confined NWs from the optimized bulk unit cells of the selected III-V compounds, and to evaluate their structural, electronic, optoelectronic properties.
3. To utilize the optimized geometry of pristine NWs for the construction and optimization of axial/radial HSNWs.
4. To compute the aforementioned properties of these HSNWs and establish a relationship between the size, shape, and material and phase dependent properties of the HSNWs for building a pathway for designing unique materials with desired properties.

Summary of Research Work

The detailed summary of the research work carried out with proposed objectives is organized and presented in form of six chapters.

CHAPTER 1 gives detailed description of the contribution of the III-V materials in the fields of the optoelectronics, nanoelectronics and thermoelectrics and the advancements made in these group of materials through modifications incorporated by means of chemical doping of the materials or through modifying the structural phase and/or imposing strain/confinement, etc. The different III-V materials like gallium nitride, gallium phosphide, gallium arsenide, gallium antimonide, boron nitride, boron phosphide, boron arsenide, etc. have significantly contributed to the field of opto-electronics to thermoelectric devices; especially, the group III-nitrides and -arsenides have become famous owing to their adaptable electro-optic transport characteristic profiles. One of the reports on GaP NWs grown with wurtzite phase suggests direct nature of electronic bandgap with magnitude 2.17 eV in contrast to its bulk counterpart.[30,31] This gap, being direct in nature, suggests its utilization in optoelectronic devices. Apart from the III-nitrides and -arsenides, the gallium antimonide based HSNWs have received scarce attention, and need to be explored owing to its high thermoelectric figure of merit in its bulk phase,[31] which can be enhanced by means of imposing dimensional confinement[32]. Apart from gallium based HSNWs, the aluminum

based pristine and HSNWs have not been studied so far for testing their application in the field of optoelectronics and thermoelectrics.

CHAPTER 2 covers the step-by-step description regarding the theory and approach utilized for studying the proposed properties of selected III-V materials under bulk and nano regimes. The first theoretical approach starting from Born-Oppenheimer approximation to the latest ground breaking electron density based approximation formulated by Walter Kohn and Sham together with different exchange-correlation functionals like local density approximation (LDA) and generalized gradient approximation (GGA) for the construction of pseudopotentials is described to get detailed account on the development of the electron density based approach. The advanced electronic structure methods like *hybrid* functionals, *GW* method, etc. for correcting the electronic band profiles are also discussed. Apart from the electronic properties, we have also evaluated the optoelectronic, vibrational and thermoelectric properties of the proposed systems and respective approaches have been included in the present chapter. The evaluation of optical transport properties has been done by computing the frequency dependent complex di-electric function of the materials that explicitly gives graphical representation of the optical transport as a function of frequency/energy thus, validating the active regime of the material within the electro-magnetic spectrum. To validate the stability of the materials and to unravel the phonon dynamics of the material, the density functional perturbation theory (DFPT) has been applied. Last but not the least, the present chapter sheds light on the Boltzmann Transport

theory utilized for evaluating electron and phonon contributions to the overall thermoelectric transport properties of the materials.

CHAPTER 3 is focused on the structural, electronic, vibrational and thermoelectric properties of the gallium pnictides,GaX (X=P/As/Sb) taking into consideration the two polytypic phases, the cubic zinc blende (ZB) and the hexagonal wurtzite (WZ). The electronic band structure calculation performed for all systems reveal direct nature of electronic bandgap except for GaP. Encouraged by the moderate and direct nature of the electronic bandgaps of these materials, and to validate their applicability to the field of thermoelectrics, the vibrational dynamics of the systems was evaluated by means of computing the phonon dispersion curves (PDCs) and phonon density of states (PHDOS). The absence of soft phonon modes and/or imaginary frequency components in the PDCs of all systems validate the dynamic stability of the systems in both polytypic phases. The PHDOS trends were utilized for assessing the thermal transport properties of the systems and, the 2^{nd} order inter-atomic harmonic force constants (IFCs) were utilized for computing the 3^{rd} order anharmonic IFCs that can be further used for solving the Boltzmann Transport equations for phonons that account for assessing phonon contributions to thermoelectric transport properties. At the end, the results on phase dependent thermoelectric properties of GaX systems show that the WZ phase, the most preferred phase at nanoscale, gives lower thermal conductivity and higher thermoelectric figure of merit (ZT) which replicate the thermoelectric efficiency of the material. Furthermore, the GaSb stands out as a promising candidate for thermoelectric

applications amongst the remaining pnictide siblings. After getting markable results on the electronic, vibrational and thermoelectric profiles of GaX compounds in WZ phase, we then constructed two-dimensionally confined one-dimensional nanostructures for understanding the modification in the properties of GaX subjected to quantum confinement. As expected, the strong quantum confinement effect results in expansion of the band edge states of all the three systems. To get deep insight into the properties of these NWs, we have re-performed all the computations by varying the size (diameter (~1, 2 and 3 nm, see Figs. 1(a, b, c))) of the NWs and by applying uniaxial external strain. These two parameters also help in tuning the properties of the NWs according to the desired application. The diameter dependent profiles of the electro-optic properties of GaX NWs suggest that the GaP NW with ~3 nm diameter shows direct nature of electronic band gap with moderate magnitude of 1.9058 eV, whereas, the remaining sibling NWs retain indirect nature of bandgap with reduction in gap magnitude as a function of NW diameter (2.27, 1.86 and 1.60 eV for GaAs NW and 1.68, 1.25 and 0.99 eV for GaSb NW, respectively). The results of strain dependent electronic responses of the NWs reveal dramatic indirect to direct bandgap transition for all three NWs at 4% uniaxial compressive strain. Furthermore, the frequency dependent complex di-electric functions are evaluated; which suggests peak absorption of electro-magnetic energy occurs within visible-ultraviolet region. Owing to these observations, the applicability of these systems can be validated in the field of optoelectronic and photovoltaic devices. On the other hand, the dramatic indirect to direct electronic phase transition at 4% uniaxial compressive strain is observed for three nanowires which suggests that these NWs can

be utilized in strain dependent switching devices. The unique electronic and optical responses of the system under bulk and nano regime provide inspiration for studying the system for thermoelectric applications.

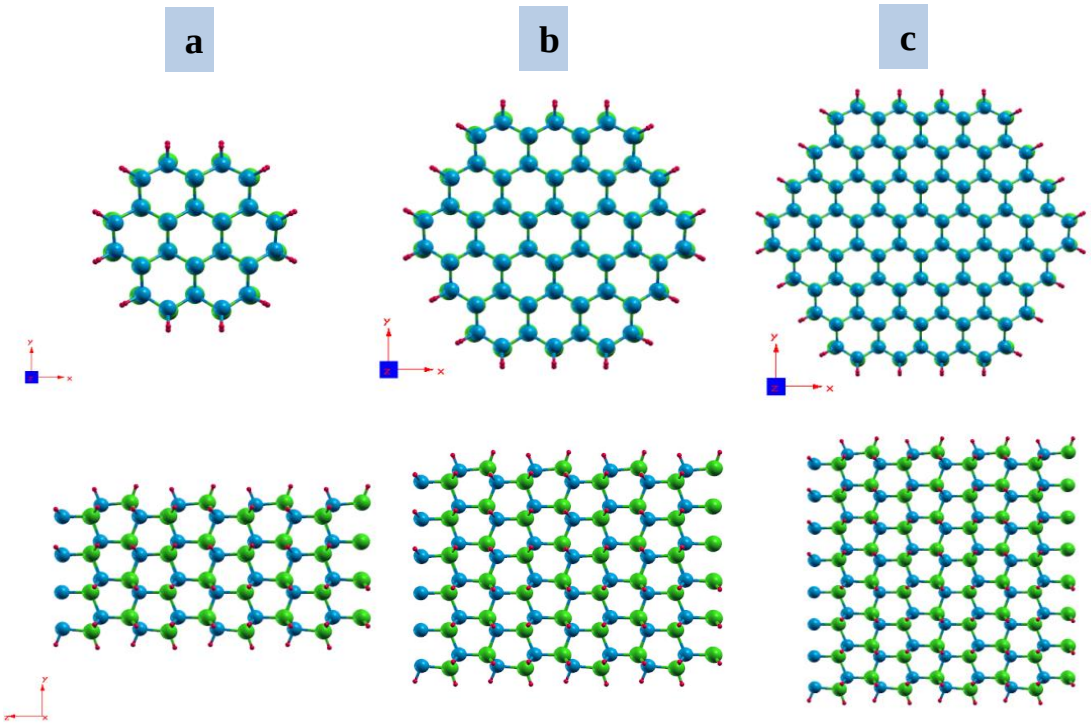

Figure 1. Top (a) and side (b) views of hydrogen saturated GaX (X=As/Sb) NWs with diameters ~1, 2 and 3 nm (The atoms in Blue, Green and Red colour represent Ga, As/Sb and H atoms, respectively).

Moving towards the main objective of the present research work, we then utilized the optimized pristine GaX NWs for constructing the radial heterostructure (HS) with core/shell (CS) geometry. The two such core/shell HSNWs namely, GaSb/GaP and GaSb/GaAs, were constructed and respective electro-optic responses were evaluated under the approach described in **CHAPTER 2** and the respective results are presented in the next chapter, **CHAPTER 4**. To study the effect of shape dependent modifications in the HSNW properties, the core NWs made up of GaP and GaAs with two distinct cross-

sectional area (round and triangular, see Figs. 2(a, b)), were embedded inside the GaSb shells making overall cross-section of the HSNWs hexagonal. The first-time studied

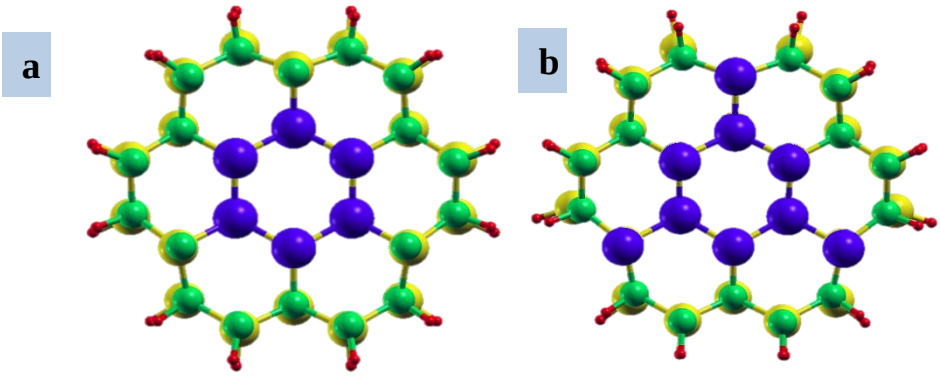

Figure 2. Cross-sectional, top (a, b) view of GaSb/GaX core-shell CS-HSNWs (X=P/As).

approach of tailoring the system properties with respect to core shape and core material could be a unique pathway for tuning the electro-optic transport through the HSNWs. This also gives opportunity to precisely modulate the charge carrier recombination rates through surface charge trapping, subjected to distinct electronic edge states of the hetero-layers (core/shell). The best way to assess the cause of the modulation in the transport and the edge states, is to evaluate the conduction and valence band edge states of the hetero-layers and assess the band alignment subjected to heterostructured geometry of the NWs. Depending on the band alignment, there are three types of heterostructures, namely, type-I, type-II and type-III. Amongst the three types, type-II heterostructure is the most preferable configuration owing to its ability to trap surface charge carriers and decrease the recombination rates. This unique characteristic is the foundation for the construction of opto-electronic devices and photovoltaic solar cells. Therefore, besides electronic and optical transport properties of the GaSb/GaP and Gasb/GaAs CSHSNWs,

we have also evaluated the solar cell parameters of these HSNWs for validating the applicability of the systems in the field of photovoltaics.

Being the most contributing materials, besides GaX compounds, we have also considered two famous aluminium based pnictide compounds namely, aluminum phosphide and aluminum arsenide for computation and to assess their structural, electronic, optical and thermoelectric properties in their bulk and confined geometries and the respective results are presented in **CHAPTER 5**. These two compounds have been reported for their markable performance for the devices utilized ranging from optoelectronics to photovoltaics[33]. Similar to the other III-V compounds, AlP and AlAs also tend to crystallize in WZ phase with hexagonal symmetry under confined geometry, despite existing in ZB phase with cubic symmetry in their bulk counterpart. To systematically study the phase dependent properties of these materials, we have first studied the bulk AlP and AlAs under the proposed approach and then the optimized unit cells of both compounds were considered for the construction of the pristine AlP and AlAs NWs. Structural to electronic to optical transport properties were computed for both NWs for the assessment of quantum confinement effect. Dramatic direct to indirect band gap transition in the case of AlAs compound was observed subjected to two-dimensional confinement; whereas, the AlP preserves its direct nature of electronic bandgap even after imposing confinement. As expected, the dimensional confinement of both compounds results in enhancement of the electronic band gap magnitude. These results indicate that the AlP under confined dimensions is suitable for opto-electronic applications owing to

its direct and moderate magnitude of bandgap. The next step in the study was to utilize these pristine NWs for constructing the axial and radial heterostructures. The two variants of radial HSNWs AlP/AlAs and AlAs/AlP were then considered for fully optimizing all the structural parameters under specific threshold criteria. The electronic and optical transport properties of the core/shell heterostructure NWs (CS-HSNWs) unravel spatially confined charge carriers owing to the desired band gap alignment. The bandgap magnitude of 2.72 eV with direct nature in the case of AlAs/AlP CS-HSNW also supports the applicability of the considered HSNW in the field of photovoltaic solar cells. On the other hand, the second variant AlP/AlAs CS-HSNW shows totally different behavior. Apart from the band alignment, the electronic band structure calculations reveal indirect nature of the bandgap with gap magnitude of 2.60 eV. Inspired by these results, we then constructed axial HSNW (A-HSNW) from AlP and AlAs, by stacking the individual unit cells of the pristine NWs on each other in 0001 direction. This constructed axial HSNW was then fully relaxed until the convergence criteria were not achieved. All proposed properties evaluated for bulk, pristine NWs and CS-HSNWs were then recomputed for the A-HSNW. The results in this case show direct nature of bandgap with type-II alignment that is of utmost importance due to its ability to reduce carrier recombination rates and increase overall efficiency. This chapter provides full-insight to the electro-optic transport properties of AlX compounds ranging from its bulk phase to the confined NW geometry to the spatially constructed radial and axial heterostructured NW configurations, and sheds light on unique pathway to engineering the carrier dynamics in the semi-conducting NWs.

The last chapter of the thesis, **CHAPTER 6** contains the results and discussion on the vibrational properties of selected III-V compounds under bulk and nano regime. The spatially originating vibrational Raman modes due to diversity in the atomic arrangements in polytypic phases of the III-V compounds have been evaluated under density functional perturbation theory (DFPT) approach[34] and supported by available data. Furthermore, the effect of nanostructuring on the vibrational properties of the compounds has been also assessed for detailed analysis of confinement dependent dynamics of the systems. Apart from the dynamic properties, the applicability of the proposed systems in one of the emerging energy application field of hydrogen generation through water-splitting process is assessed by means of computing the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) based catalytic activity of the systems under hydrogen and oxygen adsorption. The results suggest that the phosphide based group III-nanowires subjected to substitutional defected condition are more sensitive to hydrogen/oxygen adsorption and yield better catalytic activities. The results show significance of metal-free novel materials that have potential to be utilized as active HER/OER catalysts subjected to their unique properties. And further enhancement in the catalytic response can be achieved by means of tailoring the electronic bandgap of the system/s through optimizing dopant concentration and/or phase/structure engineering.

The overall results on the structural, electronic, optical, vibrational and thermoelectric properties of III-V compounds ranging from their bulk phase to nanostructured geometry

has been summarized in **CHAPTER 7**. The results show the pathway towards engineering the properties of the system by means of engineering the phase, dopant concentration, size, shape, geometry and composition. At the end, the thesis is concluded with brief description on scope of a probable future research.

References

[1] Z. Wu, J.B. Neaton, and J.C. Grossman, *Phys. Rev. Lett.* **100**, 236805 (2008).

[2] J.C. Johnson, K.P. Knutsen, H. Yan, M. Law, Y. Zhang, P. Yang, and R.J. Saykally, *Nano Lett.* **4**, 197 (2004).

[3] S.S. Lo, T.A. Major, N. Petchsang, L. Huang, M.K. Kuno, and G. V. Hartland, *ACS Nano* **6**, 5274 (2012).

[4] Y. Li, F. Qian, J. Xiang, and C.M. Lieber, *Mater. Today* **9**, 18 (2006).

[5] M. Nolan, S. O'Callaghan, G. Fagas, J.C. Greer, and T. Frauenheim, *Nano Lett.* **7**, 34 (2007).

[6] J. Tersoff, Nano Lett. **15**, 6609 (2015).

[7] S. Meister, H. Peng, K. McIlwrath, K. Jarausch, X.F. Zhang, and Y. Cui, *Nano Lett.* **6**, 1514 (2006).

[8] K.A. Dick, C. Thelander, L. Samuelson, and P. Caroff, *Nano Lett.* **10**, 3494 (2010).

[9] F. Qian, Y. Li, S. Gradečak, D. Wang, C.J. Barrelet, and C.M. Lieber, *Nano Lett.* **4**, 1975 (2004).

[10] Y. Wu, J. Xiang, C. Yang, W. Lu, and C.M. Lieber, *Nature* **430**, 61 (2004).

[11] L. Samuelson, C. Thelander, M.T. Björk, M. Borgström, K. Deppert, K.A. Dick, A.E. Hansen, T. Mårtensson, N. Panev, A.I. Persson, W. Seifert, N. Skold, M.W. Larsson, and

L.R. Wallenberg, *Phys. E Low-Dimensional Syst. Nanostructures* **25**, 313 (2004).

[12] X. Hong-yi, G. Ya-nan, L. Zhi-ming, B. Timothy, L. Hao-feng, Q. Gao, H.H. Tan, C. Jagadish, and J. Zou, *Nanoscale Res. Lett.* **7**, 589 (2012).

[13] S.K. Lim, M. Brewster, F. Qian, Y. Li, C.M. Lieber, and S. Gradečak, *Nano Lett.* **9**, 3940 (2009).

[14] X. Jiang, Q. Xiong, S. Nam, F. Qian, Y. Li, and C.M. Lieber, *Nano Lett.* **7**, 3214 (2007).

[15] Y. Hu, H.O.H. Churchill, D.J. Reilly, J. Xiang, C.M. Lieber, and C.M. Marcus, *Nat. Nanotechnol.* **2**, 622 (2007).

[16] R. Songmuang, G. Katsaros, E. Monroy, P. Spathis, C. Bougerol, M. Mongillo, and S. De Franceschi, *Nano Lett.* **10**, 3545 (2010).

[17] J. Xiang, W. Lu, Y. Hu, Y. Wu, H. Yan, and C.M. Lieber, *Nature* **441**, 489 (2006).

[18] P. Parkinson, H.J. Joyce, Q. Gao, H.H. Tan, X. Zhang, J. Zou, C. Jagadish, L.M. Herz, and M.B. Johnston, *Nano Lett.* **9**, 3349 (2009).

[19] W. Guo, M. Zhang, P. Bhattacharya, and J. Heo, *Nano Lett.* **11**, 1434 (2011).

[20] H.J. Joyce, J. Wong-Leung, C.K. Yong, C.J. Docherty, S. Paiman, Q. Gao, H.H. Tan, C. Jagadish, J. Lloyd-Hughes, L.M. Herz, and M.B. Johnston, *Nano Lett.* **12**, 5325 (2012).

[21] P. Caroff, M.E. Messing, B. Mattias Borg, K.A. Dick, K. Deppert, and L.E. Wernersson, *Nanotechnology* **20**, 495606 (2009).

[22] K.L. Kavanagh, *Semicond. Sci. Technol.* **25**, 024006 (2010).

[23] G.E. Cirlin, V.G. Dubrovskii, I.P. Soshnikov, N. V. Sibirev, Y.B. Samsonenko, A.D. Bouravleuv, J.C. Harmand, and F. Glas, *Phys. Status Solidi - Rapid Res. Lett.* **3**, 112 (2009).

[24] L.E. Fröberg, B.A. Wacaser, J.B. Wagner, S. Jeppesen, B.J. Ohlsson, K. Deppert, and L. Samuelson, *Nano Lett.* **8**, 3815 (2008).

[25] C. Himwas, S. Collin, P. Rale, N. Chauvin, G. Patriarche, F. Oehler, F.H. Julien, L. Travers, J.C. Harmand, and M. Tchernycheva, *Nanotechnology* **28**, 495707 (2017).

[26] C. Himwas, S. Collin, H.-L. Chen, G. Patriarche, F. Oehler, L. Travers, O. Saket, F.H. Julien, J.-C. Harmand, and M. Tchernycheva, *Nanotechnology* **30**, 304001 (2019).

[27] S. Zhang, A.T. Connie, D.A. Laleyan, H.P.T. Nguyen, Q. Wang, J. Song, I. Shih, and Z. Mi, *IEEE J. Quantum Electron.* **50**, 483 (2014).

[28] Y. Zhang, M. Aagesen, J. V. Holm, H.I. Jørgensen, J. Wu, and H. Liu, *Nano Lett.* **13**, 3897 (2013).

[29] W. Kohn and L.J. Sham, *Phys. Rev.* **140**, (1965).

[30] S. Assali, I. Zardo, S. Plissard, D. Kriegner, M.A. Verheijen, G. Bauer, A. Meijerink, A. Belabbes, F. Bechstedt, J.E.M. Haverkort, and E.P.A.M. Bakkers, *Nano Lett.* **13**, 1559 (2013).

[31] T.K. Gajaria, S.D. Dabhi, and P.K. Jha, *Sci. Rep.* **9**, (2019).

[32] N. Mingo, *Appl. Phys. Lett.* **84**, 2652 (2004).

[33] G. Boras, X. Yu, and H. Liu, *J. Semicond.* **40**, 101301 (2019).

[34] S. Baroni, S. De Gironcoli, A. Dal Corso, and P. Giannozzi, *Rev. Mod. Phys.* **73**, 515 (2001).

List of Publications related to Thesis

1. Gajaria, T. K., Dabhi, S. D., Baraiya, B. A., Mankad, V., & Jha, P. K. (2017, May). Vibrational properties of III-V semiconductor in wurtzite phase: A comparative density functional theory study. In *AIP Conference Proceedings* (Vol. 1832, No. 1, p. 090043). AIP Publishing.
2. Gajaria, T. K., Dabhi, S. D., & Jha, P. K. (2019). ab initio Energetics and Thermoelectric Profiles of Gallium Pnictide Polytypes. *Scientific reports*, *9*(1), 5884.
3. Gajaria, T. K., Dabhi, S. D., & Jha, P. K. (2019, July). Diameter and strain dependent structural, electronic and optical properties of gallium phosphide nanowires. In *AIP Conference Proceedings* (Vol. 2115, No. 1, p. 030178). AIP Publishing.
4. Gajaria, T. K., Roondhe, B., Dabhi, S. D., Śpiewak, P., Kurzydłowski, K. J., & Jha, P. K. (2019). Hydrogen evolution reaction electrocatalysis trends of confined gallium phosphide with substitutional defects. *International Journal of Hydrogen Energy*. (Accepted)
5. Gajaria, T. K., Roondhe, B., Dabhi, S. D., & Jha p. K., (2019). Exploring the hidden catalyst from boron pnictide family for HER and OER. *International Journal of Hydrogen Energy*. (Accepted)

List of Publications not related to Thesis

1. Gajaria, T. K., Dabhi S. D., & Jha P. K., (2019). Electro-Optic Transport through Janus Monolayers of In2SSe, In2STe and In2SeTe. In *AIP Conference Proceedings*. AIP Publishing. (Accepted)
2. Dalsaniya, M., Patel, K., Gajaria, T. K., & Jha P. K., (2019). AlC- ML. In *AIP Conference Proceedings*. AIP Publishing. (Accepted)

Date: 10/12/2019

Place: Vadodara

Signature of Candidate
(Trupti K. Gajaria)

Signature of Supervisor
(Prof. P. K. Jha)

----------*END OF SYNOPSIS*----------