Effect of Impurities on Optical and Transport Properties of Semiconducting Devices and Quantum Wires

Jitendra Kumar Paswan*

Author's Affiliations:	Assistant Professor, Department of Physics, Patna Science College, 800005, Patna University, Bihar, India.
*Corresponding author:	**Jitendra Kumar Paswan** Assistant Professor, Department of Physics, Patna Science College, 800005, Patna University, Bihar, India. E-mail: jitendrakumarpaswan481@gmail.com

ABSTRACT	The study of effect of impurities on semiconductors and quantum wires were made. The effect on conductance was increased because of chemical potential transport properties were also influenced by twist angles of bilayer graphene. Thermal conductivity was obtained by the variation of impurities and scattering rates. Fluctuation mode played a peculiar role and changed twist angles to decrease conductivity. The Monte Carlo simulation and Boltzmann transport equation were used for the calculation of results. The analysis showed a role for study of interlayer interaction. In response of microscopic transport mechanism, the conductance Eigen channels were considered for this study.
KEYWORDS	Optical and transport properties, impurity, quantum wire, chemical potential, twist angle of bilayer, phonon, Monte Carlo simulation, interlayer interaction.

INTRODUCTION

Quay et al. Studied the transport properties by the use of non-interacting electron model [1]. Pershin et al. used Landauer-Buttiker formalism for the study of transfer of electrons from one reservoir to another by the use of small bias across the channel [2]. Egues et al. presented the influences of spintonics for the study of low dimensional semiconductor systems due to electron spin [3]. Park et al. and Ganichev et al. studied that the symmetry in bulk inversioncreated quantum well electric potential on narrow gap semiconductor material surface and tuned Rashba-spin-orbit interaction [4,5]. Krstajic et al. studied quantum wire rings [6]. Sun et al. studied spin dependent transport [7]. Mireles et al. and Kumar et al. studied that the sequel affected properties semiconductor and quantum wires [8,9]. Xie analysed the effect of impurities [10]. Kokurin studied theoretically the properties of quantum wires. The electronic properties were also studied for doped nanostructure [11]. Lee et al., Zhang et al. and Guo and Wang presented heat transport phenomena using phonon hydrodynamic transport process [12,13,14]. Yu et al. studied the behavior of phonons in different materials when there was dominance of *n*-type phonon scattering [15]. Guo and Wang studied the two dimensional graphene and boron nitride in phonon hydrodynamic due to phonon characteristics of out-plane phonon mode and obtained

relation in long wavelength limit [16]. Wang et al. studied the conductivity in response to thermal transport [17]. Fan et al. made first principle calculations maintaining computational efficiency of empirical potentials using machine learning potentials process due to accuracy [18]. Lv et al. used long wavelength limit for the study of dispersion in different materials which showed linear behavior as quadratic [19]. Duan et al. studied graphene hetrostructure characteristics [20]. Lindsay et al. calculated thermal conductivity and explained phonon dissipation relations by means of neuroevolution potential, density functional theory and optimized Tersoff potential combined with the Lennard Jone potential in the case of twisted bilayer graphene structures [21,22]. Chen et al. presented approaches using Fourier's law of heat conduction for nanostructured materials and found deviations for non-Fourier heat transport phenomena [23]. Yue et al. showed that emerged machine learning potentials method was used for the study of twisted bilayers in response of hydrodynamics [24]. Kokovin et al. studied the relative magnitudes of displacement [25].

METHOD

Spintonic consideration was made for the study of the required cases. Spin polarized field effect transistor was used in the study. The spin-orbit interaction was taken for semiconducting devices. This was useful for electronic and optical characteristics of impurity in the quantum wires as transport nature of low dimensional devices were fabricated. The effect of impurities on electronic properties of bulk semiconductors were recognized. Diagonalization technique was used in this study. Wave function was

used considering the relations $k_y = \dfrac{p_y}{\hbar}$. for propagation and then it was given by the relation $\hat{H} = \hat{H}_q + \hat{H}_R$.

The energy eigen values and eigen vectors $\hat{H}_q$ was given by

$$\hat{H}_q \psi_{n\sigma}(X) = E_{n\sigma} \psi_{n\sigma}(X)$$

The calculation was made by using Landuer formation. Neuroevolution potential machine learning framework for the development of results were considered. The total energy was obtained. The central atom i and radial component were obtained by the.

$$q_n^i = \Sigma\, g_n\left(r_{i,j}\right)$$

Applied for neighbor atoms with cutoff distance, $g_n\left(r_{i,j}\right)$ is the radial function.

RESULTS AND DISCUSSION

The study of the effect of energy dispersion for conduction having many strength of impurity were made. The effect was also examined for twist angles of bilayer graphene using phonon scattering rates in response of heat transfer. Graph (1) shows the plot of energy dispersion of quantum wires versus magnetic fields. The strength of magnetic field and impurity factors were used in the study. Graph (1) (a) shows the plot of each energy level of subbands in response to dispersion in absence of electric field. A lateral shift was produced in this case. Graph (2) represented Rashbha spin orbit interaction. Coupling between the spin split levels produced anticrossing between subband became sharper. Graph (3) shows the plot of energy dispersion of quantum wires versus electric field and impurity factor. The impurity factor affected the properties of quantum wires and semiconducting devices. The change in energy dispersion produced different transport properties and was found useful for molecular and nanoscale electronic applications. The ballistic conductance's were obtained for quantum wires and semiconductors by the use of impurities. The electronic and optical characteristics in quantum wires and semiconductor were studied and it was found that transporties of low dimensional cases were affected. This was due to existence of the impurities. The effect of impurities on thermal properties and optical properties were studied and was found that in the case of twist angel of bilayer graphene. This was examined for effect of twist angle. It was found the fluctuated mode played an important role for transport properties.
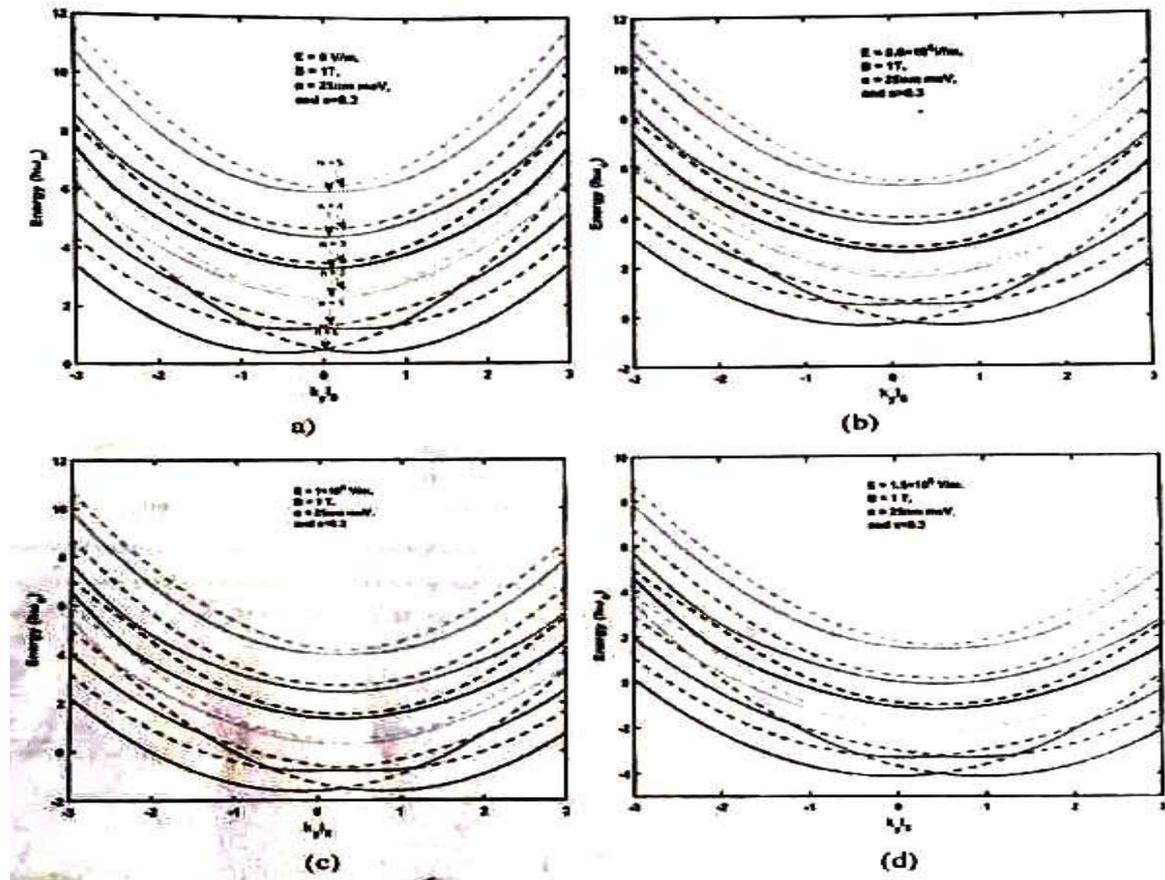
Graph 1: Plot of energy dispersion of quantum wires vs magnetic fields and impurity factors.
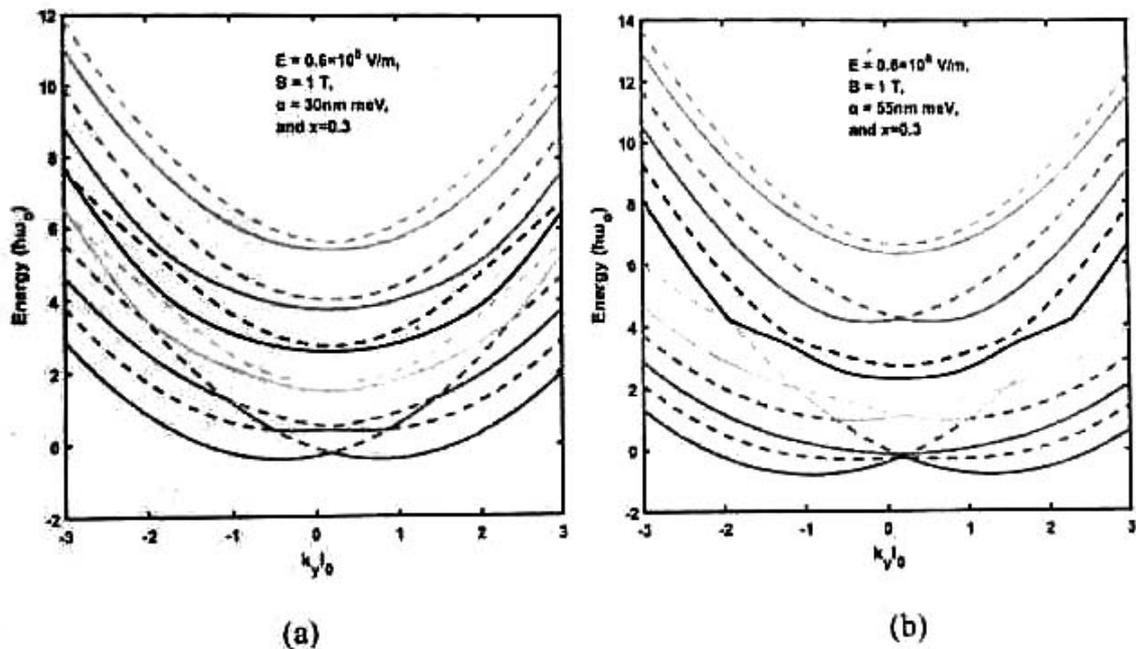
Graph 2: Plot of energy dispersion of quantum wires vs electric field and Rashba spin orbit interactions.
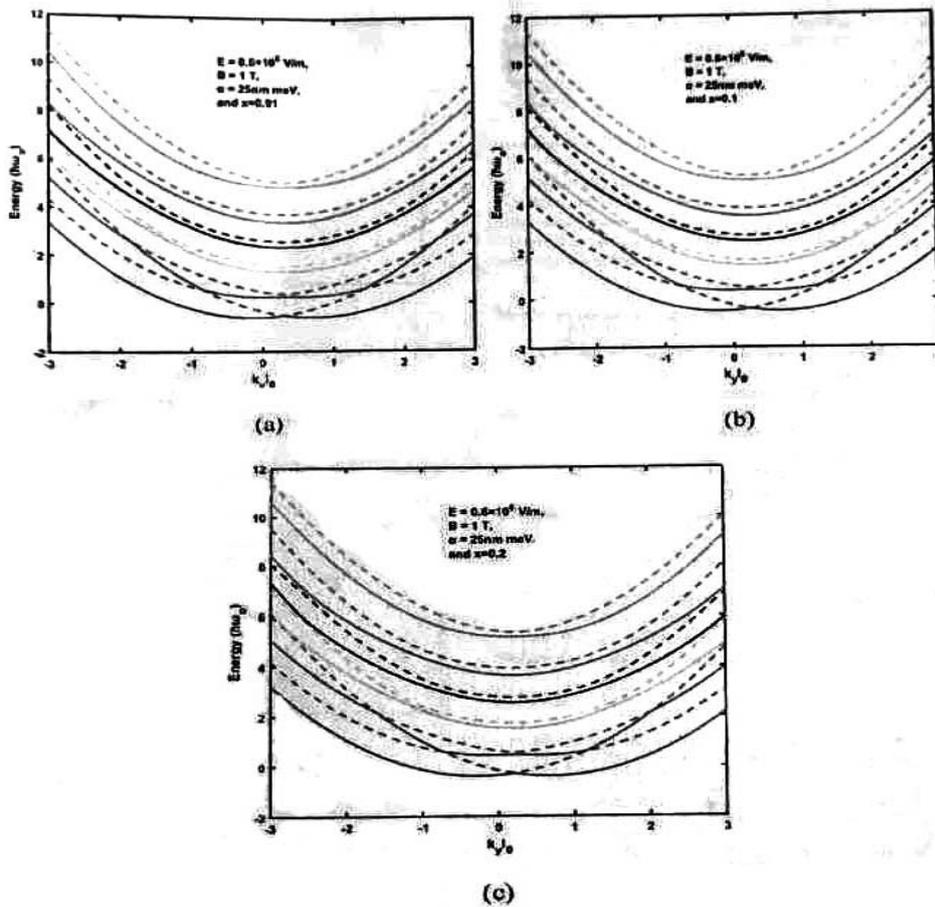
Graph 3: Plot of energy dispersion of quantum wires vs electric field and impurities.

CONCLUSION

The doped impurities affected the transport in semiconductors and quantum wires and semiconducting devices. In this study parabolic confinement was used. The cases of effects due to magnetic field were considered and examined. It was found that the electronic and optical characteristics of impurities in semiconductor and quantum wires were affected. This effect was due to existence of impurities. Energy eigen values and eigen vectors were quantized by diagonalization fluctuation in mode was found in the case of bilayer graphene due to decrease of twist angle change. This resulted implications applications and it was essential for controlling thermal conductivity.

REFERENCES

1. Quay CHL, Hughes TL, et al. Observation of one-dimensional spin–orbit gap in a quantum wire. **Nat Phys.** 2010;6:336–339.

2. Pershin YV, Shevchenko SN, Vagner ID, Wyder P. Electronic transport through a nuclear spin polarization–induced quantum wire. **Phys Rev B.** 2002;66:205309.

3. Egues JC, Burkard G, Loss D. Datta–Das transistor with enhanced spin control. **Appl Phys Lett.** 2003;82:2658–2660.

4. Park YH, Kim HJ, et al. Separation of Rashba and Dresselhaus spin–orbit interactions using crystal-direction-dependent transport measurements. **Appl Phys Lett.** 2013;103:1063.

5. Ganichev SD, et al. Experimental separation of Rashba and Dresselhaus spin splittings in semiconductor quantum wells. **Phys Rev Lett.** 2004;92:256601.

6. Kraštić PM, Pagano M, Vasilopoulos P. Transport of low-dimensional semiconductor structures in the presence of spin–orbit interaction. **Phys E Low Dimens Syst Nanostruct.** 2011;43:893–900.

7. Sun QF, Wang J, Guo H. Quantum transport theory for nanostructures with Rashba spin–orbit interaction. **Phys Rev B.** 2005;71:165310.

8. Mireles F, Kirczenow G. Ballistic spin-polarized transport and Rashba spin

precession in semiconductor nanowires. **Phys Rev B.** 2001;64:024426.

9. Kumar M, Lahon S, Jha PK, Gumber S, Mohan M. Spin–orbit interaction effect on nonlinear optical rectification of quantum wires in the presence of electric and magnetic fields. **Phys B Condens Matter.** 2014;438:29–34.

10. Xie W. Impurity effects on optical properties of a spherical quantum dot in the presence of an electric field. **Phys Rev B.** 2004;69:045323.

11. Kokurin LA. Effect of spin–orbit coupling on spectral and transport properties of tubular electron gas in InAs nanowires. **Phys E Low Dimens Syst Nanostruct.** 2015;74:264–270.

12. Lee S, Broido D, Esfarjani K, Chen G. Hydrodynamic phonon transport in suspended graphene. **Nat Commun.** 2015;6:6290.

13. Zhang Z, Ouyang Y, Guo Y, Nakayama T, Nomura M, Volz S, et al. Hydrodynamic phonon transport in bulk crystalline polymers. **Phys Rev B.** 2020;102:195302.

14. Guo Y, Wang M. Phonon hydrodynamics and its applications in nanoscale heat transport. **Phys Rep.** 2015;595:1–44.

15. Yu C, Shan S, Lu S, Zhang Z, Chen J. Characteristics of distinct thermal transport behaviors in single-layer and multilayer graphene. **Phys Rev B.** 2023;107:165424.

16. Guo Y, Wang M. Heat transport in two-dimensional materials by directly solving the phonon Boltzmann equation under Callaway's dual relaxation model. **Phys Rev B.** 2017;96:134312.

17. Wang Y, Dai H, Liu Z, Liu D. Van Hove singularity modulation of phonon transport in bilayer graphene. **J Phys Chem C.** 2023;127:23752–23760.

18. Fan Z, Zeng Z, Zhang C, et al. Neuroevolution machine-learning potentials: combining high accuracy and low cost in atomistic simulations and applications to heat transport. **Phys Rev B.** 2021;104:104309.

19. Lv B, Hu X, Wang N, Song J, Liu X, Gao Z. Thermal transport properties of novel two-dimensional nitride phosphorus: an *ab initio* study. **Appl Surf Sci.** 2021;559:149463.

20. Duan F, Shen C, Zhang H, Qin G. Hydrodynamically enhanced thermal transport due to strong interlayer interactions: a case study of strained bilayer graphene. **Phys Rev B.** 2022;105:125406.

21. Lindsay L, Broido DA. Optimized Tersoff and Brenner empirical potential parameters for lattice dynamics and phonon thermal transport in carbon nanotubes and graphene. **Phys Rev B.** 2010;81:205441.

22. Liu W, Hong Y, Zhang J, Yue Y. Anisotropic thermal transport in twisted bilayer graphene. **Phys Chem Chem Phys.** 2022;24:21722–21730.

23. Chen R, Hu S, Ren W, Zeng C. Modulating phonon transport in bilayer black phosphorus: unraveling the interplay of strain and interlayer quasi-covalent bonds. **Phys Rev B.** 2024;109:165413.

24. Yue J, Hu S, Xu B, Chen R, Xiong L, et al. Unraveling the mechanisms of thermal boundary conductance at the graphene–silicon interface: insights from ballistic, diffusive, and localized phonon transport regimes. **Phys Rev B.** 2024;109:115302.

25. Kokovin AD, Burmistrov IS. Attenuation of flexural phonons in freestanding crystalline two-dimensional materials. **Phys Rev B.** 2024;110:125432.

****