Twist modulated Electronic band gap & Carriers Mobility of Graphene Helical.

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ABSTRACT

We have investigated the electronic band structure and carrier mobility of three types of AGNRs (N=6, 7 & 8) using Density functional theory combined with Deformation potential theory and Effective mass approximation. It is shown that all AGNRs are direct gap semiconductors or semi-metallic, except twisted N=6 FAGNRs. N=6 & 7 have moderate or low carrier mobility comparable to that of graphene. Nevertheless, for N=8 the hole and electron carriers mobility is high of the order of 4.43x10^3 and 7.55x10^3 cm^2V^-1m^-1 respectively for untwisted HAGNRs which decrease with increase in torsional angle magnitude. Similar response has been noticed for N=8 FAGNRs. Our results suggest that twisting in ribbon can be considered as a more controllable way for manipulating the band structure and carriers mobilities for applications in mechanical switch devices.

1. Introduction

For understanding of the transport and optical properties of graphene nanoribbons, an unambiguous determination of their electronic band structure is necessary. The calculated band gap value by using GGA-PBE functional[1] underestimates the measured band gap values[2,3] of pi-conjugated systems. Despite that the determination of other properties like effective mass[4,5] or work function[6] is observed to be in excellent agreement with experimental study. Although, even after several attempts to explains the reason of significant variation in the band gap values, like image charge correction approximation[3] or effects of length[7], it remains an unsettled issue, yet, the variation in the measured values of effective masses has been explained by Boris et. al. in which the measured values meets excellently with calculated values obtained by Density functional theory (DFT) using GGA-PBE functional[5]. Moreover, as also reported in case of Phosphorene’s nano ribbons that the effective masses determined by the PBE functional are more and sufficiently close to the measured value than by the HSE06
functional, allow us to be confident in the ability to calculate the effective mass and carriers mobility with reasonable accuracy[8]. This motivates us to study the effect of twisting of armchair graphene nanoribbons (AGNRs) on the band structure and effective mass.

In this paper, we studied not only the effect of twisting but also the effect of passivation on electronic bands and its curvature-dependent property i.e. effective mass of a twisted armchair of a bipartite lattice GNRs[9–12] within the fixed boundary condition making translational symmetry tractable only for a few discrete twist angles values (θ). It is to be mentioned that the use of periodic boundary condition (PBC) for helical shaped GNRs allows only discrete torsional deformations compatible with the translational symmetry along Z-direction, opens up route to inquire the role of symmetry on the band structure which helps extract the physics of 1D material in the nature. The systematic study of the narrow GNRs prototypes for N= 6, 7 and 8 each separated into basically three groups with a hierarchy of band gap response to torsional strain (θ) (i.e. Families of AGNRs with number of dimers equal to $q=3N$ have quadratic monotonous increasing response to torsion strain, for $q=3N + 1$ the band gap monotonously decreases, while the family with $q=3N+2$ the band gap decreased or smaller values of torsional strain and then increases) given by $q = \text{mod}(N, 3)$ [13], $N$ is number of dimer lines across the ribbons width ($W$). Because -(i) for wider AGNRs the three families are very close to each other yet substantial changes has been reported for the narrowest ribbons with $W<1 \text{ nm}$[13] also (ii) the computational limitations- were the reason that restricted our investigation to the GNRs to narrow width in order to forms the helical shaped morphologies with small number of atoms. We considered most frequent H-terminated AGNRs (HAGNRs) and F-terminated AGNRs (FAGNRs) each planar ribbon has four categories of topology that can be described on the basis of their respective inversion and mirror symmetries[14] and we chose (i) zigzag' type termination with N=odd have both mirror and inversion symmetry and (ii) zigzag termination with N=even have only mirror symmetry. Our DFT calculations predict
the electronic and transport properties of helical shaped AGNRs within PBC at discrete torsional angles. Remarkably, the method of incorporating PCB allows determining the properties based on band structure and the effect of symmetry properties on energy eigenvalues for simulated helical shaped AGNRs under selected discrete twist values with fixed rigid ends. Absence of axial ionic relaxation allows us to study the helical with axial effective strain resulting from twisting as well as torsional strain simultaneously.

2. Computational Details

All the calculations presented in this work are performed using spin-polarized first-principles method by using SIESTA simulation package. Normconserving Troullier Martin pseudo potential in fully separable Kleinman and Bylander form has been used to treat the electron-ion interactions. The exchange and correlation energies have been treated within both GGA-PBE functional. The Kohn Sham orbitals were expanded as a linear combination of numerical pseudo atomic orbitals using a split-valence double zeta basis set with polarization functions (DZP). All atomic positions and lattice constants are optimized by using the conjugate gradient method, where the total energy and atomic forces are minimized. The convergence for energy is chosen as $10^{-5} eV$ between two steps. Throughout geometry optimization, the confinement energy of numerical pseudo-atomic orbitals is taken as 0.01 Ry. Minimization of energy was carried out using standard conjugate-gradient (CG) technique. Converged values of sampling for the k-mesh grid $\sim 10^{-2} \text{Å}^{-1}$ have been used according to Monkhorst-Pack scheme to sample Brillouin zone.

The structures were relaxed until the force on each atom was less than $10^{-2} eV\text{Å}^{-1}$. The spacing of the real space used to calculate the Hartree exchange and correlation contribution of the total energy and Hamiltonian was 800Ry for untwisted AGNRs and the converged values in a range between 1300Ry to 1450Ry was taken for twisted AGNR. Vacuum region of about
~12Å along perpendicular to periodic Z-direction were used in calculations to prevent the superficial interactions between the periodic images.

3. Results and Discussion

It is worthwhile to discuss our previous study[19] in which we have calculated the lattice parameters for pristine unit cells of HAGNRs and FAGNRs that were found to be in good agreement with the previously reported values (Table 2). The lattice constants of untwisted N=6 H passivized AGNR (HAGNRs), N=7 HAGNRs and N=8 HAGNRs are found to be 4.325Å, 4.316Å and 4.321Å respectively. We multiply the unit cell to form a super cell and twist the AGNRs mechanically by π-rad to form helical morphologies and then performed the ionic relaxation only, refraining from any axial relaxation. The fixed end condition does not allow any axial contraction i.e. the inverse Poynting effect[20] and mechanically twisting the one end produce the helical shaped conformation as we have shown schematically the

| Table 1: Comparision of measured and Calculated band gaps (in eV) for the untwisted pristine N=6, 7 and 8AGNRs. |
|---|---|---|---|
| 6-HGNARs | 7-HGNARs | 8-HGNARs |
| 1.11 | 1.66 | 0.43 | ref[1] PBE |
| 1.12 | - | 0.20 | ref[21] PBE |
| 1.34*, 1.02# | 1.27*, 1.57# | 0.01*, 0.25# | ref[22] TB*, LDA# |
| - | 2.3 | - | ref[7] TDFT-PBE0 |
| 1.12*, 2.68# | 1.62*, 3.81# | 0.30*, 1.15# | ref[23] LDA*, GW# |
| - | 1.6 | - | ref[24] Exp. |
| - | 2.5±0.1 | - | ref[25] Exp. |
| - | 2.3±0.1*, 3.7# | - | ref[3] Exp.*, GW# |
| - | 2.7 | - | ref[26] Exp. |
| - | 2.62*, 1.67# | - | ref[27] Exp.*, PBE# |
| 1.14 | 1.49 | 0.20 |
| Our Results PBE |
transition of planar AGNR (Figure 1(a)) to helical shaped conformation (Figure (2b)). Further increase in torsional angle decreased the unit cell size $L_M$ while increasing the torsional strain as again demonstrated in the transition from (Figure (2b)) to (Figure (2c)). Likewise we have modeled and studied these few discrete torsional angles compatible with translation symmetry along Z-direction for HAGNRs and FAGNRs.

Figure 1: Schematic description of mechanics of twisting that has been applied to the infinite long (a) planar GNR with minimum lattice constant $L_M$=Å and torsional angle $\theta$=zero that morphs it into (b) helical shaped infinite long twisted AGNR with increased value lattice constant $L_M$=Å and torsional angle $\theta$=zero that eventually shrinks to (c) the helix with much smaller lattice constant when gets more twisted. The $L_m$ is the lattice constant shown in cell, $W$ is the width of AGNR and $\gamma_{max}$ is the angle between the rotation axis $\theta$ (pointing outward to this page) with the tangent to the curve joining the edge atoms.

We classified these different helical conformations by three parameters shown in Figure 1: lattice constant ($L_M$), torsional angle($\theta$), width ($W$) of AGNRs as given in the Table 2. The subscript $M$ of lattice constant $L_M$ is the number of times unit cell get repeated or multiplied to have required twisted super cell.
3.1. Electronic properties

To have an insight into the electronic band structure of H & F AGNRs, we have performed band structure calculations. Because electromechanical response of twisted helical can be understood in a unified way by using the notion of effective strain, therefore we will discuss the observable response only to effective strain in the rest of the article. The effective strain 

\[ \varepsilon_{\text{eff}} = \theta^2 \Sigma^2 \]  

[28] i.e. effective tensile strain associated with the twist angle \( \theta \) and \( \Sigma^m = 2 \int_0^{W/2} \rho^{m-1} d\rho; \ 0 \leq \rho \leq W/2 \), where the width (\( W \)) of the ribbons at each twist is given in Table 2. The calculations reveal that among the untwisted AGNRs, the narrowest ones 6 H & F AGNR have the highest band-gap of 1.14eV and 1.41eV respectively, effectively making it a semiconductor. On applying the torsional strain the band gap increased monotonously in case of N=6 HAGNRs up to 2.01eV for extreme torsional strain which is the highest band gap among all the cases we have taken. But in case of N=6 FAGNRs band gap does not vary much (See Figure 2). It is interesting to note that the basic trend of band-gap hierarchy that separates the untwisted GNRs into three groups given as 3N+1>3N>3N+2, becomes 3N>3N+2>3N+1 even for moderately twisted helical AGNRs.

![Figure 2: Except 6-FAGNRs the monotonous response of band gap to effective strain. N=7 and 8 showing linear response too.](image-url)
The direct band gap symmetry point of untwisted HAGNRs although shifted from $I$ to $\pm K$

direct $\rightarrow$ indirect band gap shifting is observed (Figure 3). In contrast the 6-FAGNRs

where $\theta=0.207 \text{rad} \AA^{-1}$

yet remains direct for all helical conformation except the most twisted for $\theta=0.207 \text{rad} \AA^{-1}$
rapidly becomes indirect band gap semiconductor even for lower value of torsional strain (Figure 4).

Likewise for N=8 H and F AGNRs helical conformations the response of the band gaps to effective strain vary monotonously as well as linearly with positive slope. Also, in these cases all the bands gaps are direct but interestingly no shift has been observed and band gap remain at $\Gamma$ point (Figure 5 and Figure 6). In effective strain space the trend of band gap response to torsional strain suggested the monotonous increasing behavior for $N=6 \& 8$ HAGNRs (i.e. $q=3N \& q=3N+2$), categorizing them into a one family. However, because of the effect of quantum size the band gap of $N=6$ AGNRs have larger band gap values.

For $N=7$ H and F AGNRs case, the response of band gaps to the effective torsional strain as we have seen in N=8 case, is monotonous and linear however have negative slopes Figure 2. This kind of response categorize the $N=7$ AGNR (i.e. $q=3N+1$) into different family. The band gaps in case of untwisted 7-H and F AGNRs are direct at $\Gamma$ point (Figure 7a and Figure 8a)), that shifted to $\pm K$ but remains direct even for higher torsional strain Figure 7(b to f) and

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**Figure 7:** Calculated spin polarized band structure of (a) Untwisted hydrogen passivized edges of 7-AGNR) with zero torsional strain per unit radial distance ($\gamma / \rho$). Band structure for the torsional strain value (b) 8.33 (c) 6.94 (d) 5.95 (e) 5.20 (f) 4.63. The VBM and the CBM to measure the band gap value for each system is marked with blues arrows.

**Figure 8:** Calculated spin polarized band structure of (a) Untwisted fluorine passivized edges of 7-AGNR) with zero torsional strain per unit radial distance ($\gamma / \rho$). Band structure for the torsional strain value (b) 8.33 (c) 6.94 (d) 5.95 (e) 5.20 (f) 4.63. The VBM and the CBM to measure the band gap value for each system is marked with blues arrows.
Table 2: Structural parameters Lattice constant ($L$) in Å, Torsional angle ($\theta$) in $^\text{rad}$ Å, Band gap ($E_g$) in eV, Effective masses ratio, hole mobility ($\mu_{1D}^h$) and electron mobility ($\mu_{1D}^e$) in $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ and width ($W$) in Å. Results of previous studies shown in brackets.

|       | $L$  | $\theta$ | $E_g$ | $m^*_h/m_e$ | $m^*_e/m_e$ | $\mu_{1D}^h$ | $\mu_{1D}^e$ | $W$  |
|-------|------|-----------|-------|-------------|-------------|--------------|--------------|------|
| 6-HAGNR | 4.325 | Zero      | 1.144 | -0.17       | 0.17        | 317.94       | 378.92       | 6.147 |
|        | 32.439 | 0.097     | 1.437 | -0.18       | 0.18        | 298.34       | 346.89       | 6.133 |
|        | 28.114 | 0.112     | 1.524 | -0.19       | 0.19        | 266.68       | 325.98       | 6.123 |
|        | 23.789 | 0.132     | 1.651 | -0.22       | 0.21        | 213.76       | 265.22       | 6.110 |
|        | 19.464 | 0.161     | 1.852 | -0.24       | 0.2319      | 190.78       | 232.73       | 6.085 |
|        | 15.139 | 0.207     | 2.011 | -0.41       | 0.32        | 86.26        | 144.58       | 6.030 |
| 7-HAGNR | 4.316 | Zero      | 1.493 | -0.40       | 0.46        | 129.04       | 85.88        | 7.365 |
|        | 34.525 | 0.091     | 1.164 | -0.34       | 0.31        | 162.82       | 153.73       | 7.324 |
|        | 30.209 | 0.104     | 1.081 | -0.29       | 0.29        | 204.22       | 167.04       | 7.307 |
|        | 25.894 | 0.121     | 0.963 | -0.27       | 0.29        | 227.21       | 171.32       | 7.274 |
|        | 21.578 | 0.146     | 0.797 | -0.24       | 0.21        | 283.47       | 280.45       | 7.224 |
|        | 17.262 | 0.182     | 0.548 | -0.18       | 0.20        | 431.10       | 293.84       | 7.131 |
| 8-HAGNR | 4.310 | Zero      | 0.198 | -0.05       | 0.05        | 4976.92      | 8411.9588    | 8.634 |
|        | 36.720 | 0.086     | 0.276 | -0.05       | 0.05        | 4427.47      | 7549.84      | 8.574 |
|        | 32.325 | 0.097     | 0.336 | -0.06       | 0.06        | 3207.53      | 5469.03      | 8.564 |
|        | 28.015 | 0.112     | 0.452 | -0.08       | 0.09        | 2088.67      | 3351.72      | 8.535 |
|        | 23.705 | 0.132     | 0.631 | -0.12       | 0.13        | 1190.95      | 1784.30      | 8.493 |
|        | 19.395 | 0.162     | 0.898 | -0.19       | 0.20        | 612.18       | 950.87       | 8.420 |
| 6-FAGNR | 4.443 | Zero      | 1.407 | -0.18       | 0.17        | 1400.20      | 887.46       | 6.068 |
|        | 33.322 | 0.094     | 1.543 | -1.05       | 0.35        | 103.19       | 296.48       | 6.059 |
|        | 28.879 | 0.109     | 1.539 | -1.39       | 0.23        | 67.09        | 546.56       | 6.052 |
|        | 24.436 | 0.128     | 1.533 | -1.36       | 0.21        | 69.41        | 607.36       | 6.046 |
|        | 19.933 | 0.157     | 1.526 | -1.20       | 0.32        | 84.29        | 332.1345     | 6.020 |
|        | 15.55 | 0.202     | 1.517 | -1.12       | 0.40        | 92.94        | 240.98       | 5.967 |
| 7-FAGNR | 4.421 | Zero      | 0.926 | -0.24       | 0.24        | 365.53       | 231.24       | 7.263 |
|        | 35.368 | 0.089     | 0.658 | -0.15       | 0.15        | 704.35       | 437.19       | 7.239 |
|        | 30.947 | 0.101     | 0.608 | -0.13       | 0.13        | 863.28       | 535.99       | 7.222 |
|        | 26.526 | 0.118     | 0.520 | -0.14       | 0.14        | 838.84       | 520.4153     | 7.194 |
|        | 22.105 | 0.142     | 0.355 | -0.10       | 0.10        | 1374.52      | 853.15       | 7.141 |
|        | 17.684 | 0.178     | 0.048 | -0.02       | 0.02        | 11661.10     | 7220.05      | 7.043 |
| 8-FHGNR | 4.411 | Zero      | 0.319 | -0.06       | 0.06        | 1448.48      | 4286.64      | 8.540 |
|        | 37.494 | 0.084     | 0.595 | -0.11       | 0.10        | 636.45       | 2006.99      | 8.510 |
|        | 33.083 | 0.095     | 0.654 | -0.13       | 0.12        | 498.76       | 1563.20      | 8.494 |
|        | 28.672 | 0.110     | 0.748 | -0.15       | 0.15        | 392.99       | 1142.93      | 8.469 |
|        | 24.261 | 0.129     | 0.912 | -0.19       | 0.19        | 276.30       | 803.86       | 8.424 |
|        | 19.850 | 0.158     | 1.186 | -0.25       | 0.28        | 176.55       | 440.34       | 8.351 |
Figure 8(b to f). In case of N=7 & 8 it is visibly obvious in Figure 2 to see that the passivation with F shifts the band gap response to effective strain downward without altering the trend. In Table 2 we have given the calculated band gap values and band gaps. For untwisted AGNRs the calculated results are consistent to those reported in previous theoretical studies as shown in Table 1. The anomalous behavior of N=6 AGNRs can be understood through our previous study[19] in which we calculated the charges on H and F atoms $\Delta Q = 0.022e$ and $\Delta Q = -0.030e$ respectively that are not observed to vary on twisting and insignificantly vary (|0.002|) on varying dimer number $N$. Hence suggests that for narrower N=6 FAGNRs the electron density depletion from carbon skeleton is comparatively more.

Furthermore, because of the downward shift of approximate value ~0.5eV in the band gap values of 7-FAGNRs w.r.t. 7-HAGNRs the Dirac cone has come to appear at $\pm K$ point. This allow the electrons with high momentum flow dissipation less through the strongly twisted 7=FAGNRs at low bias in contrast to the results of 8 H and F AGNRs in which the untwisted nano-ribbons shows Dirac cone at $\Gamma$ point allowing the electrons with low momentum flows dissipation less through. Hence, passivation along with torsional strain play decisive role in the semimetal-to-semiconductor or semiconductor-to-semimetal transformation.

3.2. Effective Mass & Mobility

The expression linking the electrical conductivity to the carriers’ mobility is $\sigma = e\mu_{1D} n = ne^2\tau/m^*$, where $\mu_{1D}$ is the mobility and $m^*$ is the effective mass. If no change in the timescale $\tau$ for quasiparticle occurs, then the mobility is inversely proportional to the effective mass, whereas, especially for large torsional angle the scattering time may be altered which influence the mobility of carriers. Detail investigation of that is beyond the scope of present work. Nevertheless, we explore another way to calculate the carriers’ transport by applying
deformation potential (DP) theory and effective mass approximation. The DP has been obtained as \( E_1 = dE_{Edge}/d\varepsilon_{eff} \) where \( dE_{Edge} \) is the energy of the valance band maxima (VBM) for holes or the conduction band minimum for electrons. Within the elastic limits the magnitude of DP describes the degree interaction between electrons and phonons. Therefore, lower value of DP indicates a weaker electron phonon hence increase in the mobility of electrons (holes). Accordingly, for 1D systems the carriers’ mobility is \( \mu_{1D} = ne\hbar^2C_{1D}/(2\pi k_B T)^{\frac{1}{2}} |m^*|^{3/2}E_1^2 \), where \( T=300K \), and \( C_{1D} \) is the stretching modulus caused by uniaxial strain which has been calculated using the expression \( C_{1D} = \frac{1}{L_0} \frac{d^2}{d\varepsilon^2}E_S \) in which \( E_S \) is the strain energy of a unit cell. In case of parabolic band the effective mass is related to how the band energy \( (E_{nk}) \) varies with the wave vector \( (k) \) by \( m^* - 1 = \hbar^2 \partial^2 E_{nk}/\partial k^2 \) captures much of the physics of carrier transport.

![Graph](image)

**Figure 9**: Energy–strain relationship along armchair (a) HAGNR and (b) FAGNR. The variation of difference in strain energy \( (\Delta E) \) with uniaxial strain \( (\varepsilon) \) applied along the armchair directions are shown in **Figure 9**. Based on those energy-strain curves we have obtained the line-stiffness \( C_{1D} \) given in **Table 3**. The values of \( C_{1D} \) are greater for FAGNRs than HAGNRs counterparts.
Figure 10: Shifts of electron affinity (χ) and ionisation potential (ξ) under effective torsional strain. The dashed lines are the linear fitting.

Figure 10 shows the shifts of band edges (E_{Edge}) i.e. electron affinity (χ) and ionisation potential (ξ) as a function of effective torsional strain along the armchair direction. Through twisting the AGNRs along the armchair directions, the DP constant \( E_i \) is then calculated as \( dE_{Edge}/d\varepsilon \), equivalent to the slope of the fitting lines, where \( E_{Edge} \) is the energy of the conduction (valence) band edge. The \( E_i \) values of Hand F AGNRs are shown in Table 3. Except N=6 FAGNRs, the standard deviation of all \( E_i \) values is smaller than 1% excluding three values marked in Table 3.

Table 3: The line stiffness (\( C_{1D} \)) and deformation potential (\( E_i \)) of Hydrogen and Fluorine passivated AGNRs.

|            | \( C_{1D} \) \((10^{10} \text{ eV/m})\) | \( E_i \) of electron \((\text{eV})\) | \( E_i \) of hole \((\text{eV})\) |
|------------|-----------------------------------------|-------------------------------------|---------------------------------|
| 6HAGNR     | 3.72                                    | 1.1492                              | -1.06572                        |
| 7HAGNR     | 4.49                                    | -1.045                              | 1.15606                         |
| 8HAGNR     | 5.10                                    | 0.90546                             | -0.69339                        |
| 6FAGNR     | 4.06                                    | -0.53999                            | -0.726114                       |
| 7FAGNR     | 4.82                                    | -0.94485                            | 1.199123                        |
| 8FAGNR     | 5.27                                    | 1.246292                            | -0.73067                        |
On the basis of obtained energy band spectrum and calculated values of $E_i$ and $C_{id}$ we determined the acoustic phonon-limited mobility at room temperature (300 K). The results are shown in Table 1. The responses of electron and holes mobilities are shown in the Figure 11. Our results show the response of twisting for N=7, the $m_h^*/m_e$ decrease from 0.40 to 0.18 for HAGNRs and 0.24 to 0.02 for FAGNRs. Similar decreasing trend is observed for the $m_e^*/m_e$ values as it decreased from 0.46 to 0.20 for HAGNRs and 0.24 to 0.02 for FAGNRs.

![Figure 11](image)

**Figure 11**: The response of (a) holes and (b) electron effective mass to effective torsional strain.

Whereas, for N=6 & 8 HAGNRs and N=8 FAGNRs, the effective mass increased as a response to increase in effective strain. For instance the values of $m_h^*/m_e$ for N= 8 increased from 0.046 to 0.18 for HAGNRs and from 0.06 to 0.25 for FAGNRs. The value of effective mass for FAGNRs are lower to its HAGNRs counterpart and also the sensitivity for twisting is more in the case of FAGNRs. Our results show that the $m^*$ for electrons and holes in untwisted N=7 HAGNRs are 0.39 and 0.46 $m_e$, respectively, which are in good agreement with Senkovskiv et al[5] and Söde et al[4]. Furthermore, it is clearly seen that the $|m^*|$ of hole for N=6 FAGNRs,
for even a small magnitude of twisting, became heavier than the \(|m^*|\) of electron significantly, which means that the carrier transport ability of electron is very strong.

The electron mobilities for N=6, 7 and 8 untwisted H & F AGNRs are about 378.92, 85.88 and 8411.96 & 887.46, 231.24 and 4286.64 cm²V⁻¹s⁻¹, respectively. The corresponding hole mobilities of untwisted H & F AGNRs are about 317.94, 129.04 and 4976.92 & 1400.20, 365.53 and 1448.48 cm²V⁻¹s⁻¹, respectively. For N=6 and 7 case, the mobilities of carriers of F passivated AGNRs is significantly higher than H passivated AGNRs. However, in case of N=8, the mobilities of H passivated AGNRs is greater than F passivated AGNRs. As a response to twisting the carriers mobilities get increased in case N=7 AGNRs. The most twisted configuration of N=7 FAGNRs has the highest value of carrier mobilities among all the cases we considered due to the Dirac cone formation at extreme twist. It is clear from the Figure 12 that N=8 HAGNRs has the most sensitive and monotonous response to torsional strain. Also it has the best electron carrier transmitting capacity and the biggest difference between the electron and hole mobility among all considered cases.

**Figure 12:** The response of (a) hole mobilities and (b) electron mobilities to effective torsional strain.
4. Conclusion

In summarily, we have calculated the electronic band structures and the intrinsic charge carrier mobilities H and F passivated AGNRs of three type AGNRs, and the effect of twisting on them, using first-principles density functional theory and the DP theory. We find that all H and F AGNRs are direct gap semiconductors or semi-metallic can have transition from semiconductor-to-metallic or metallic-to-semiconductor state. Direct semiconductor state of N=6 FAGNRs turns to indirect semiconductor state on moderate twisting. Band structure calculations of N=7 AGNRs show that the reduction of band gap value as well as the effective mass as a response to twisting which eventually turn out to be a Dirac cone at the extreme twisting point in case of FAGNRs. The numerical results indicate that the electron mobilities varies moderately in case of N=6 and N=7 AGNRs but, in case of N=7 the response to twist is very strong. The electron mobility in case of N=8 HGNRs & FAGNRs at room temperature decreased from 8411.96 to 950.87 & 4286.64 to 440.34 cm2V−1s−1, respectively as a response to twist, is higher than the corresponding hole mobility. However, the mobilities of carriers increased in case of N=7 moderately.

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