Spin polarization in lateral two-dimensional heterostructures

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Abstract
In this work, we study the spin polarization in the MoS(Se)2–WS(Se)2 transition metal dichalcogenide heterostructures by using the non-equilibrium Green’s function method and a three-band tight-binding model near the edges of the first Brillouin zone. Although it has been shown that the structures have no significant spin polarization in a specific range of energy of electrons, by applying a transverse electric field in the sheet of the metal atoms, shedding light on the sample, and under a small bias voltage, a significant spin polarization in the structure could be created. Besides, by applying a suitable bias voltage between leads and applying the electric field, a noticeable spin polarization can be found even without shedding the light on the heterostructures.

Keywords: spin polarization, lateral heterostructure, transition metal dichalcogenides

(Some figures may appear in colour only in the online journal)

1. Introduction

By decreasing the minimum feature size of electronic devices, the charge-based ones encounter some limitations including power dissipation and the manufacturing cost. There are different strategies for overcoming these kinds of limitations. Beyond the Moore strategy, scientists have tried to substitute not only novel materials instead of silicon but also the spin degree of freedom instead of the charge of an electron. After discovering the single atomic layer of graphite, called graphene [1], due to some graphene boundaries, scientists tried to discover and use the graphene-like two-dimensional materials as an alternative to the conventional three-dimensional semiconductors for manufacturing electronic devices. Transition metal dichalcogenides (TMDs) with general formula as MX2 (M = Mo, W and X = S, Se) are one group of them. TMDs have fascinating and unique properties such as strong spin–orbit coupling (SOC) in the valence band edge, the number of layers dependent bandgap, higher absorption coefficient per unit thickness as compared to conventional semiconductors [2], long spin lifetime [3–6], and strong excitonic effects [7]. Regarding the strong spin–orbit coupling, significant conduction and valence band spin splitting, and very long electron spin lifetimes, TMDs are one of the main candidates for manufacturing the spin-based devices [8–10] and many scientific groups are trying to improve the specifications of TMDs. For instance, Guo et al., have used doping techniques to enhance the spin splitting in the monolayer of WS2 [3]. It has been shown that the spin relaxation time is enhanced by a small in-plane magnetic field in the monolayer of WSe2 [11]. Komsa et al., tuned the bandgap and in consequence the spectral region of MoS2/MoSe2/MoTe2 compounds by alloying [12]. Based on the assertion of another group, the size and direct-indirect bandgap in the WX2 (X = S, Se, and Te) monolayer can be altered by strain engineering technique [13]. Stability enhancement of MoS2 by changing its phase from 2H to 1T through Li intercalation is the subject of reference [14]. Forming stacked MX2 (M = Mo, W and X = S) heterostructures can be altered by strain engineering technique as it has been asserted in reference [15] is a way to expedite electron–hole separation for photonic applications. Besides, some references have reported a correlation between the formation of heterostructures and altering the photocatalytic and optical properties of TMDs [7, 16].
In the process of fabricating electronic devices, a homo-
junction is created by doping an impurity in the semicon-
ductor materials while a heterojunction, as the basis of het-
erostructures, is made by using two semiconductors with
different energy gaps. Generally, TMD heterostructures are
divided into two lateral and vertical groups. At least two lay-
ers of different TMD monolayers are needed to be stacked
and form a vertical (planar) heterostructure. Similarly, if
the layers stitch beside each other, a lateral (in-plane) hetero-
structure can be formed. In this regard, various groups have been
reported practical achievement of sharp and defect-free lat-
eral heterostructures via different methods such as lateral epiti-
taxial and thermal CVD processes [6, 14, 17]. This is while
improving the interfacial properties of the heterostructures by
means of various methods is still in progress [6]. A wide
range of TMD based applications has been reported so far, e.g.
in-plane transistors, diodes, p-n photodiodes, and com-
plementary metal-oxide-semiconductor (CMOS) inverters [6].
Furthermore, optoelectronic applications of van der Waals
(vdW) and lateral heterostructures are increasing due to the
rapid interlayer charge transfer [18] and type engineering abil-
ity [6]. Heo et al. have reported a rotation-based interlayer
photocexcitation in MoS2/WS2 monolayer stacks due to the in-
direct to direct transitions [19]. Likewise, the enhancement of
photoexcited charge carriers separation and collection through
photovoltaic structure under lateral and vdW heterostructures
was carried out by Atwater et al. [2].

A fine review on spintronic in two-dimensional materi-
als and their heterostructures can be found in reference [20].
It has been shown that the heterostructures can significantly
improve the SOC [20]. Some examples are graphene with a
WS2 substrate, TLs/graphene vdW heterostructure, and MoS2
on the graphene channel [20]. Zhang et al. have reported
high-spin polarization at room temperature in 2D layers by
reducing its carrier lifetime via the construction of vdW het-
erostructures. A near-unity degree of spin polarization has
been observed in PbI2 layers with the formation of type-I and
type-II band aligned vdW heterostructures with monolayers of
WS2 and WSe2 [21]. Zhou et al. have studied the vdW
graphene/hafnene heterostructure with different stacking con-
figurations and shown that the distinct electronic distribution
and spin-polarized characteristic of the vdW heterostructures
come from the intensity of orbital overlap induced by diverse
stacking configurations [22]. Deyan et al. have reviewed and
discussed some of the distinctive effects observed in ferromag-
netic junctions with prominent 2D crystals such as graphene,
hexagonal boron nitride, and TMDs and showed how the spin
interface phenomena at such junctions affects the observed
magnetoresistance in devices [23]. By referring to other avail-
able references like references [24–26], one can study more
about different applications of TMD heterostructures as well
as perfect spin and valley polarization in some TMD-based
monolayers.

Using the non-equilibrium Green’s function (NEGF)
method, spin polarization in lateral MoX2–WX2 (X = S, Se)
heterostructures has been studied by our team in this paper.
Besides, the domination of W (Mo)-atom orbitals on the neg-
ative (positive) energy range of electrons for both types of the
spin degree of freedom, and the main role of d,3 orbital of both
W- and Mo-atoms in the quantum conductance of the device
under the equilibrium condition (no bias voltage between
leads) have been revealed by our studies. Under equilibrium
condition and without applying a transverse electric field and
sheding light on the structure, no significant spin polariza-
tion was seen when the energy of an electron was less than
−0.1 eV. On the other hand, under the non-equilibrium condi-
tion plus applying the field and shedding light on the sample,
in a specific range of electron energy, due to the breaking of
the time-reversal symmetry (TRS), a significant spin polariza-
tion was seen in both MoSe2–WSe2 and MoS2–WS2 lateral
heterostructures. In addition, it has been shown, the d,3 orbital
of edge atoms plays the main role in the quantum conductance
of the device under the cited condition. In consequence, we
show that a significant spin polarization can be seen in some
TMD heterostructures under special conditions and give a gen-
eral positive answer to the probable future application of the
spin degree of freedom in the TMD heterostructures [24–26],
as it has been demonstrated that a heterostructure can improve
the SOC [27]. It is worth noting, up to our best knowledge, the
spin polarization in lateral TMD heterostructures haven’t been
studied theoretically and experimentally. In consequence, we
can not compare our results with others.

The structure of this article is as follows. The material
parameters and calculation methods are provided in sections 2
and 3, respectively. Section 4 includes the results and discur-
sion, and in section 5 one can read the summary.

2. Material parameters

The honeycomb configuration of the MoS(Se)2–WS(Se)2
TMD heterostructures which are illustrated in figure 1 are
composed of three sections including the left lead, right
lead, and channel. In our calculations, the channel area
which is divided into two MoS(Se)2 and WS(Se)2 semi-
finite nanoribbons at the left and right side appropriately,
consists of 72 metal atoms. Note that the mismatch
between the two semi-infinite nanoribbons is negligible [28].
Figure 1(c) presents the next nearest neighbor atoms for a cen-
tral metal atom. The magnitude of each displacement vector,
\( \vec{R}_i \), is calculated

\[
\hat{R}_i \propto \sum_{i=1}^{6} \hat{R}_i \propto \sum_{i=1}^{6} \vec{R}_i
\]

in that figure equals 3.19 \( \AA \) (3.34 \( \AA \) for
MoS(Se)2–WS(Se)2 heterostructure. It must be emphasized,
in the numerical calculations, we only consider the metal
atoms with a triangular lattice structure, and in consequence,
electrons only hop between the metal atoms in six different
directions.

3. Calculation method

Exploiting a three-band Hamiltonian model [29–34] and
the NEGF method, besides the spin polarization studies in lateral
two-dimensional MoS(Se)2–WS(Se)2 TMD heterostructures,
it has been shown, at the two K and K’ corners of first Bril-
louin zone, the Bloch states in monolayer MX2 (M = Mo, W
and X = S, Se) mostly consist of \( d_{\gamma} \) orbital for the conduc-
tion band minimum (CBM), and \( d_{\gamma} \) and \( d_{\gamma} \) for the valence

\[
d_{\gamma} \] and \( d_{\gamma} \) for the valence
Figure 1. Schematic of MoS(Se)2–WS(Se)2 TMD heterostructure (a) top view, (b) left lead side view, (c) next nearest neighbor atoms for each central metal atom. $\vec{R}_i$ ($i = 1, \ldots, 6$) are the displacement vectors. The lattice constant and the length of each $\vec{R}_i$ vector are equal to 3.19 Å (3.34 Å) in MoS(Se)2–WS(Se)2 heterostructure.

band maximum (VBM) [5, 35–39]. Additional information including the hopping matrix between metal atoms in each displacement direction and the on-site matrix of each metal atom is provided in appendix A. In order to calculate the spin polarization and spin current which are defined as equations (1) and (2) respectively, one should evaluate the transmission probability, $T^+$, of spin up (down) electrons through the NEGF method [40–43].

$$SP = \frac{T^+ - T^-}{T^+ + T^-}. \tag{1}$$

$$I^{\pm}(E, V) = \frac{q}{\pi\hbar} \int T^{\pm}(E, V)[f_1(E, V) - f_2(E, V)]dE. \tag{2}$$

In equation (2), $h$, $q$, $E$, $V$, and $f_{1,2}$ refer to the reduced Planck constant, elementary charge of electron, energy, potential, and Fermi distribution function of leads, respectively. Near the equilibrium condition, by shedding the light on the channel, some electrons are excited to higher energy levels and their energy increases by $\hbar\omega$ where $\omega$ is the frequency of the incident light. After a while, they come back to lower energy levels due to losing the same energy. In consequence, we are calculating the effect of the incident light on the quantum conductance of a two-level system [40] in which the energy of its electrons is equal to $E \pm \hbar\omega$. Using Fermi’s golden rule [44], one can calculate the electron–photon coupling matrix and consequently the self-energy of incident light to implement the influence of it on the system. This could be done by adding the mentioned self-energy to the Green’s function of the electrons similar to the effect of leads and their self energies (appendix B). Although the detailed information about incident light self-energy calculations exists in appendix B, a brief explanation is provided in the continuation of this paragraph. In the first step, the electron and hole correlation functions and the initial value of carrier’s density are calculated by using the Green’s function of the channel and self-energies of leads without shedding the light (zero self-energy of the photon). By means of the coupling matrix and correlation functions, one can calculate the initial value of photon self-energy which is used for evaluating the new amount of the Green’s function of the channel and the self-energy of the photon. Using Poisson’s equation, the loop is repeated until the convergence is achieved i.e., it is a self-consistent method (appendix B) in accordance with figure 2.

Since the transverse electric field is applied in the plane of metal atoms, its effect is added to the diagonal elements of the Hamiltonian matrix as a potential term. The mentioned term is calculated by multiplying the strength of the field to the $y$-coordinate of each atom while the lower (upper) edge of the nanoribbon is considered as the reference line. In addition, the bias voltage between leads changes the Fermi distribution function at left (right) lead equal to $f(E + V_{DS}/2)$($f(E - V_{DS}/2)$ where $V_{DS}$ is bias voltage. The difference between these two distributions i.e., $[f(E + V_{DS}/2) - f(E - V_{DS}/2)]$ should be considered in calculating the transmission probability [40]. It should be noted, both the bias voltage and shedding light, place the system in the non-equilibrium condition. Thus, the self-consistent method should be used for calculating the transmission probability and spin polarization [40]. It is important to note that we used the optimal values for the energy of photons, intensity of light, and the intensity of $E_T$, $E_y$ which are 0.12 eV, 20 nW μm$^{-2}$, and 0.2 eV, respectively in our mentioned numerical calculations. In other words,
we found that, by altering the mentioned parameters, the spin polarization could be changed. Therefore, at first, we calculated the optimum values for them aimed at getting the maximum spin polarization and then the optimal values were exploited in our calculations.

4. Results and discussion

Figures 3(a) and (b) show the spin up localized density of states (LDOS) for MoS$_2$–WS$_2$ and MoSe$_2$–WSe$_2$ TMD heterostructures under equilibrium condition, respectively. As these figures show, the LDOS of Mo (W)-atom dominates on the positive (negative) range of energy of electrons. Although we found that, by altering the mentioned parameters, the spin polarization could be changed. Therefore, at first, we calculated the optimum values for them aimed at getting the maximum spin polarization and then the optimal values were exploited in our calculations.

4. Results and discussion

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Figure 4. Quantum conductance of MoS(Se)$_2$–WS(Se)$_2$ for (a) spin-up and (b) spin-down electrons, under equilibrium condition.

by using density functional theory Kang et al, have shown that the highest occupied molecular orbital belongs to W-atom and the lowest unoccupied molecular orbital belongs to Mo-atom [45], because of considering the molecular orbitals of metal atoms, our results differ from their results. DOS which is the summation of LDOSs, is shown in the dashed line in figures 3(a) and (b) for MoS$_2$–WS$_2$ and MoSe$_2$–WSe$_2$ heterostructures accordingly. Based on the figures, one can say that the DOS is zero for $-0.1$ to $0.2$ eV electron energy range in MoS$_2$–WS$_2$ and $-0.02$ to $0.02$ eV in MoSe$_2$–WSe$_2$ heterostructures. In consequence, it is expected that a transmission gap will be seen in the curve of the quantum conductance.

To calculate the quantum conductance of MoS$_2$–WS$_2$ and MoSe$_2$–WSe$_2$ TMD heterostructures for both spins in accordance with figures 4(a) and (b) respectively, we used the
DOS of the system. As the mentioned figures show, when the energy of an electron, $E_e \geq -0.25$ eV, a small difference is seen between the conductance of spin-up electrons and spin-down ones. Correspondingly, a transmission gap equals to 0.3 (0.04) eV is seen in MoS$_2$–WS$_2$(MoSe$_2$–WSe$_2$) heterostructure. This implied that both nanoribbons are narrow bandgap semiconductors. Based on the curve of spin polarization under equilibrium condition as figure 5, for $E_e \geq -0.25$ eV, spin polarization is not zero, generally. For a better understanding of the role of atomic orbitals on the quantum conductance, we show the magnitude of LDOSs for spin-up electrons as circles on the lattice position of each atom (figure 6). As the figure shows, the $d_z^2$ orbital of all atoms has the main role in the quantum conductance not only on W-side but also on Mo-side. According to figures 6(a) and (b), the appeared difference in the quantum conductance curves can be attributed to the different roles and the radius of blue circles on the position of W and Mo atoms which are placed at the upper edge of a nanoribbon. Figure 7 shows the LDOS after shedding the light on the sample. Comparing figure 7 with figure 6, one can conclude that the LDOS decreases due to the occupation of states by excited electrons, probably. It should be noted, in order to have a good view of LDOS changes in the presence of light as well as make the mentioned comparison possible, the circles’ diameters are illustrated about four times larger than the calculated amounts.

Creating spin polarization in a structure could be done by implementing an external factor such as electric field [46], magnetic field [25, 47, 48], exchange field [49], or bias voltage [50] and consequently breaking TRS. With that mean, first, we apply a bias voltage at a range from $-4$ to $4$ V and a transverse electric field equal to 0.2 eV and calculate the spin-dependent current. As the spin-dependent current versus bias voltage curve in figure 8 shows, for some values of bias voltage, the spin-dependent current is not zero and therefore, the spin polarization has a non-zero value. A negligible value of the spin polarization for both MoS$_2$–WS$_2$ and MoSe$_2$–WSe$_2$ heterostructures in energies from 0.41 eV to 0.45 eV has been achieved (see figure 5). Moreover, as presented in figure 8, for $-0.1$ V $\leq V_{DS} \leq 0.1$ V, the spin-up current is equal to spin down current approximately. Now, a question can be asked. Is it possible under these conditions i.e., $0.41$ eV $\leq E_e \leq 0.45$ eV and $-0.1$ V $\leq V_{DS} \leq 0.1$ V, in which the non-zero spin polarization changes to a significant spin polarization value under shedding the light on the channel and applying a transverse electric field ($E_T$)?
As illustrated in figure 9, which is the curve of spin polarization versus the energy of electrons, when $V_{DS} = 0.1 \, \text{V}$, $E_{T,y} = 0.2 \, \text{eV}$, and the channel is under shedding the light with 20 nW $\mu \text{m}^{-2}$ intensity and 0.12 eV energy, a significant and almost constant spin polarization is seen for $0.42 \leq E_e \leq 0.44 \, \text{eV}$. It means that the answer to the above question is positive when the MoSe$_2$–WSe$_2$ heterostructure is considered. While, in accordance with figure 10, with shedding light on the channel of MoS$_2$–WS$_2$ heterostructure, a non-zero spin polarization can be seen.

To clarify the subject with regard to the influence of SOC in VBM and CBM degeneracy, spin-valley dependency, and optical selection rule in W(M)X$_2$ monolayers [51], one can say that the light excites the electrons from non-degenerate VBM to non-degenerate CBM based on the spin-valley dependency and optical selection rule. In the excitation process by the light the difference between the density of spin-up and spin-down electrons changes and in consequence, it is expected that a non-zero spin polarization is seen. As figure 9 shows, when the energy of an electron, $E_e$, is approximately in a range from 0.42 to 0.44 eV, the spin polarization in a MoSe$_2$–WSe$_2$ heterostructure has a nearly constant positive value (0.6 to 0.8) due to the domination of spin-up carriers while $E_{T,y} = 0.2 \, \text{eV}$,
Exploiting the NEGF method and three-band Hamiltonian

5. Summary

Exploiting the NEGF method and three-band Hamiltonian model, we studied the spin polarization in MoS2–WS2 and MoSe2–WSe2 lateral heterostructures. Under the equilibrium conditions, It was shown that non-significant spin polarization happens when the energy of an electron \( E_0 \) is from 0.42 to 0.44 eV, in both heterostructures, whereas applying a transverse electric field, bias voltage, and shedding light on the MoSe2–WSe2 structure, a significant spin polarization was seen for 0.42 eV \( \leq E_0 \leq 0.44 \) eV. Conversely, it was shown that a significant spin polarization happens only by shedding the light on the bias-less heterostructure while a transverse electric field exists.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Tight-binding details

The Bloch states in monolayer MX2 (M = Mo, W and X = S, Se) mostly consist of \( d_{2z} \) orbitals for CBM, and \( d_{xy}, d_{xz}, d_{yz} \) for the VBM [5, 35–39]. Therefore, by considering the base functions \( \Phi_1 = d_{2z}, \Phi_2 = d_{xy}, \Phi_3 = d_{yz} \) the next nearest tight-binding Hamiltonian [35] can be written as equation (A.1)

\[
H_{NN}(K) = \begin{pmatrix}
    h_0 & h_1 & h_2 \\
    h_1^* & h_{11} & h_{12} \\
    h_2^* & h_{12}^* & h_{22}
\end{pmatrix}.
\]  

(A.1)

Each element of \( H_{NN} \) is a 3 \( \times \) 3 matrix that represents the hopping integrals [52]. These hopping integrals change in the different displacement directions which are shown in figure 1(c). The hopping matrices are as (A.2) to (A.4) relations [52].

\[
h(R_i) = \begin{pmatrix}
    t_0 & t_1 & t_2 \\
    -t_1 & t_{11} & t_{12} \\
    t_2 & -t_{12}^* & t_{22}^*
\end{pmatrix} = h(R_4)^i, \quad (A.2)
\]

\[
h(R_4) = \begin{pmatrix}
    t_0 & t_1 & t_2 \\
    -t_1 & t_{11} & t_{12} \\
    t_2 & -t_{12}^* & t_{22}^*
\end{pmatrix} = h(R_4)^i. \quad (A.3)
\]

Therefore, the three-band TB Hamiltonian will be rewritten as relation (A.5):

\[
H = \begin{pmatrix}
    h_D & \cdots & h(R_4) \\
    \vdots & \ddots & \vdots \\
    h(R_4) & \cdots & h_D
\end{pmatrix} \quad (A.5)
\]

where,

\[
h_D(\text{up}) = \begin{pmatrix}
    \epsilon_1 & 0 & 0 \\
    0 & \epsilon_2 & i\lambda \\
    0 & -i\lambda & \epsilon_2
\end{pmatrix}, \quad (A.6)
\]

\[
h_D(\text{down}) = \begin{pmatrix}
    \epsilon_1 & 0 & 0 \\
    0 & \epsilon_2 & -i\lambda \\
    0 & i\lambda & \epsilon_2
\end{pmatrix}. \quad (A.7)
\]

The constants of the above equations are defined in table 1 [34].

Appendix B. Light interaction

The retarded Green’s function \( G^R \) is defined as:

\[
G^R = [(E + i\eta)\mathbf{I} - H_0 - \Sigma_{l1} - \Sigma_{l2} - \Sigma_{\text{photon}}]^{-1}. \quad (B.1)
\]

Where \( \eta \) equals 1.5 \( \times \) 10⁻³, \( \mathbf{I} \) is the unit matrix, \( \Sigma_{l1,2} \) are self-energy of leads, and \( \Sigma_{\text{photon}} \) is photon self-energy. The effect of leads on the channel appears as shifting the energy levels and broadening the energy level. It is assumed, due to the energy of photons, \( h_0 \), the energy of electrons changes as \( E + (h_0) \) and \( E - (h_0) \) under shedding the light on the channel, and in consequence, similar to the leads the effect of photons can be added to the Hamiltonian of the system as a self-energy. In order to evaluate the mentioned self-energy, in the first instance, we assumed that the self-energy of a photon in that equation is zero. This allows us to calculate the initial value of \( \rho \) by:

\[
\rho = dE[\text{diag}(f_L \ast G^R \ast \Gamma_{l1} \ast G^\Lambda) + \text{diag}(f_R \ast G^R \ast \Gamma_{l2} \ast G^\Lambda)]. \quad (B.2)
\]

Where, \( f_{LR} \) and \( \Gamma_{l1,2} \) are Fermi distribution function and broadening matrix of electrodes, respectively. Using equation (B.3) one can calculate the preliminary value of photon self-energy

\[
\Sigma_{\text{photon}} = \frac{i[\Sigma_{\text{in photon}} + \Sigma_{\text{out photon}}]}{-2}. \quad (B.3)
\]
Table 1. GGA based three-band TB model parameters of monolayer MX₂ in the unit of eV [34]

|       | ϵ₁   | ϵ₂   | t₀   | t₁   | t₂   | t₁₁  | t₁₂  | t₁₂₂ | λ     |
|-------|-------|-------|------|------|------|------|------|------|-------|
| MoS₂  | 1.046 | 2.104 | -0.184 | 0.401 | 0.507 | 0.218 | 0.338 | 0.057 | 0.073 |
| MoSe₂ | 0.919 | 2.065 | -0.188 | 0.317 | 0.456 | 0.211 | 0.290 | 0.130 | 0.091 |
| WS₂   | 1.130 | 2.275 | -0.206 | 0.567 | 0.536 | 0.286 | 0.384 | -0.061 | 0.211 |
| WSe₂  | 0.943 | 2.179 | -0.207 | 0.457 | 0.486 | 0.263 | 0.329 | 0.034 | 0.228 |

Where Σ^\text{in}_\text{photon}$ and Σ^\text{out}_\text{photon}$ are defined [42] as:

\[
Σ^\text{in}_\text{photon} = \sum_{pq} M_{lp} * M_{qm} * \left[ NG_{pq}^p(E - \hbar \omega) + (N + 1)G_{pq}^p(E + \hbar \omega) \right], (B.4)
\]

\[
Σ^\text{out}_\text{photon} = \sum_{pq} M_{lp} * M_{qm} * \left[ NG_{pq}^p(E + \hbar \omega) + (N + 1)G_{pq}^p(E - \hbar \omega) \right], (B.5)
\]

Where $M_{pq}$, $N$, $G^{(p)}$, and $\hbar \omega$ are electron–photon coupling matrix, number of photons, electron (hole) correlation function, and energy of photons, respectively. With the aim of calculating the proper value of photon self-energy, we have to calculate the potential of the system through Poisson’s equation as:

\[
U = (-\rho) / P. (B.6)
\]

Where $P$ is the discretized Poisson operator (appendix C). Finally, we compare the new potential value with the initial one. If their difference is bigger than a specific arbitrary value, we guess the new self-energy of photon and substitute it in equation (B.1). This self-consistent loop continues until the mentioned potential difference satisfies the mentioned requirements.

Appendix C. Poisson’s equation

Poisson’s equation in Cartesian geometry has a form like equation (C.1).

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + f = 0. (C.1)
\]

With the aim of changing the Cartesian geometry to triangular one, three new vectors called $u$, $v$, and $w$ vectors as shown in figure 11 are defined. It should be noted, in the lattice of metal atoms is triangular and in consequence, the angles $\alpha$ and $\beta$ are equal to 60 and 120 degrees, respectively. Therefore, the equation (C.1) can be written as [53]:

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{2}{3} \left( \frac{\partial^2 u}{\partial u^2} + \frac{\partial^2 u}{\partial v^2} + \frac{\partial^2 u}{\partial w^2} \right). (C.2)
\]

Using the finite difference method, the equation (C.2) can be discretized and equation (C.3) will be found [54]:

\[-6\Phi_{i,j} + \Phi_{i,j-2} + \Phi_{i,j+2} + \Phi_{i+1,j+1} + \Phi_{i-1,j+1} + \Phi_{i+1,j-1} + \Phi_{i-1,j-1} = Q_{i,j} + O(\delta^6). (C.3)\]
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