

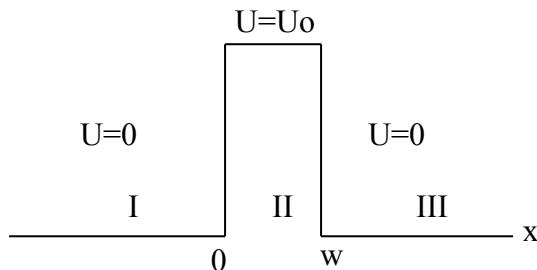
EE396V HW 2

Submit homework online on canvas. Due Monday September 23 at class time.

Show full derivation/code and results in order to get the proper credit.

#1: Electron Facing a Mountain (25 points)

Electron scattering by a potential barrier: A simple model to illustrate the ideas of reflection and transmission.



Consider the potential barrier shown above.

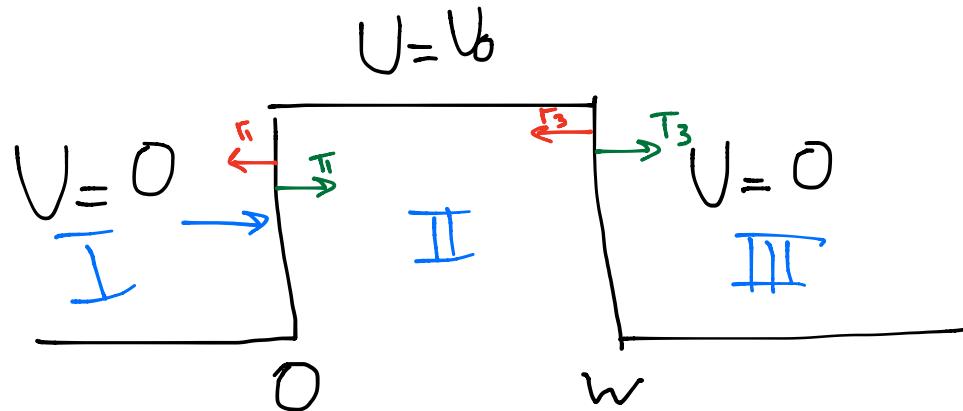
- Write the general solution for the electron wavefunction for each region (I,II,III). Note that the wavevector will be different in each region. Denote the wavefunction and wavevector in each region by ψ_i and k_i , where i is either I, II, or III.
- What is the mathematical relationship between k_I and k_{III} ?
- What is the expression for the k in each region in terms of the energy of that region?
- Now let's consider an electron in region I traveling towards the barrier with energy $E > U_0$. We want to determine the fraction of the electron that makes it through the barrier, a very important concept characteristic of all wave phenomena. What are the boundary conditions at $x=0$ and $x=w$?
- From the boundary conditions determine the transmission and reflection probabilities which are respectively defined as:

$$T = \left| \frac{\Psi_{III}^+}{\Psi_I^+} \right|^2, \quad \Gamma + T = 1$$

- For a barrier potential and width of $U_0=0.3\text{eV}$ and $w=1\text{nm}$, plot the transmission probability.
- Assuming the electron was a classical particle like a ball, and the potential barrier can be thought of as a wall, in this case sketch the transmission probability of the classical particle and compare it with your result from f). What is the key difference if any?

EE 396V - Homework 2

1. Electron Facing a Mountain:



a) TISE $\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + U(x) \Psi(x) = E \Psi(x)$

In region I, $U(x)=0$, so:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi_I(x) = E \Psi_I(x)$$

$$\Psi_I(x) = A \exp(i k_I x) + B \exp(-i k_I x)$$

$$k_I = \frac{\sqrt{2mE}}{\hbar}$$

In region II, $U(x)=U_0$, so:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi_{\text{II}}(x) + U_0 \Psi_{\text{II}}(x) = E \Psi_{\text{II}}(x)$$

$$\Psi_{\text{II}}(x) = C \exp(i k_{\text{II}} x) + D \exp(-i k_{\text{II}} x)$$

$$k_{\text{II}} = \frac{\sqrt{2m(E-U_0)}}{\hbar}$$

In region III, $U(x)=0$, so:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi_{\text{III}}(x) = E \Psi_{\text{III}}(x)$$

$$\Psi_{\text{III}}(x) = E \exp(i k_{\text{III}} x) + F \exp(-i k_{\text{III}} x)$$

However, in region III, there is no reflected wave propagating towards the $-x$ direction. Therefore, we can set $F = 0$. We therefore have:

$$\Psi_{\text{III}}(x) = E \exp(i k_{\text{III}} x)$$

$$k_{\text{III}} = \frac{\sqrt{2mE}}{\hbar}$$

$$b) k_I = k_{III}$$

$$c) k_I = \frac{\sqrt{2mE}}{\hbar} \quad k_{II} = \frac{\sqrt{2m(E-V_0)}}{\hbar} \quad k_{III} = \frac{\sqrt{2mE}}{\hbar}$$

$$d) \text{ B.C. } @ x=0 \Rightarrow ① \Psi_I(0) = \Psi_{II}(0)$$

$$\Rightarrow ② \left. \frac{d\Psi_I(x)}{dx} \right|_{x=0} = \left. \frac{d\Psi_{II}(x)}{dx} \right|_{x=0}$$

$$\text{B.C. } @ x=w \Rightarrow ③ \Psi_{II}(w) = \Psi_{III}(w)$$

$$\Rightarrow ④ \left. \frac{d\Psi_{II}(x)}{dx} \right|_{x=w} = \left. \frac{d\Psi_{III}(x)}{dx} \right|_{x=w}$$

e) From ① $\rightarrow \Psi_I(0) = \Psi_{II}(0)$

$$A + B = C + D$$

From ② $\rightarrow \frac{d}{dx} \left. \Psi_I(x) \right|_{x=0} = \frac{d}{dx} \left. \Psi_{II}(x) \right|_{x=0}$

$$A i k_I \exp(i k_I x) - B i k_I \exp(-i k_I x) = C i k_{II} \exp(i k_{II} x) - D i k_{II} \exp(-i k_{II} x)$$

$$i k_I (A - B) = i k_{II} (C - D)$$

From ③ $\rightarrow \Psi_{II}(w) = \Psi_{III}(w)$

 Note that $k_I = k_{III}$

$$(C \exp(i k_{II} w) + D \exp(-i k_{II} w)) = E \exp(i k_I w)$$

$$\exp(i k_{II} w) (C + D) = E \exp(i k_I w)$$

From ④ $\rightarrow \frac{d}{dx} \left. \Psi_{II}(x) \right|_{x=w} = \frac{d}{dx} \left. \Psi_{III}(x) \right|_{x=w}$

$$(i k_{II} \exp(i k_{II} w) - D i k_{II} \exp(-i k_{II} w)) = E i k_I \exp(i k_I w)$$

$$T = \left| \frac{\Psi_{III}^+}{\Psi_I^+} \right|^2 = \frac{k_{III}}{k_I} \frac{|E|^2}{|A|^2} = \frac{|E|^2}{|A|^2}$$

$$T = \frac{|E|}{|A|^2}$$

$$\Gamma = 1 - T$$

$$\Gamma = 1 - \frac{|E|^2}{|A|^2}$$

#2: Bravais lattice of TMDs (20 points)

This exercise is to determine the Bravais lattice of TMDs. TMDs exhibit a wide variety of crystal structures (polytypes) because an individual MX₂ monolayer, which itself contains three layers of atoms (X–M–X), can be in either one of the two phases (so called 1T or 1H phases). Most commonly encountered polymorphs are 1T, 2H (2H is the same as 1H if it is a monolayer) and 3R where the letters stand for trigonal, hexagonal and rhombohedral, respectively, and the digit (1, 2 or 3) indicates the number of X–M–X units in the unit cell (that is, the number of layers in the stacking sequence). Here, we will not dwell too much on the technical details of the crystal structure, our focus is on the Bravais lattice. For the following questions, visit the chemtube websites for the 3D dynamic view of the 2T (same as 1T if monolayer) (TaS₂ in <http://www.chemtube3d.com/solidstate/SS-MS2.htm>), and 2H (<http://www.chemtube3d.com/solidstate/SS-MoS2.htm>) crystal structure. Answer the following questions.

- a. Sketch the top-view projection of the 1T crystal structure. Use different colors or atom sizes to distinguish between metal and chalcogen atoms
- b. Draw two different primitive unit cells for that lattice. How many atoms are there per cell?
- c. Repeat a) for the 2H structure.
- d. Repeat b) for the 2H structure.
- e. Give an example of a TMD that is normally in the i) 1T structure, ii) 2H structure, and iii) 3R structure.

This question requires some literature studies.

#3: 1D Tight-binding model (20 points)

The goal of this exercise is to provide some mathematical fluency in the tight-binding formulation. Consider a 1D periodic arrangement of identical atoms with spacing a between the atoms. We will assume that every atom has one available electron. Note that this is a reasonable model for an electron in the *s* orbital. Furthermore, assume that the solutions for the atomic orbitals are known.

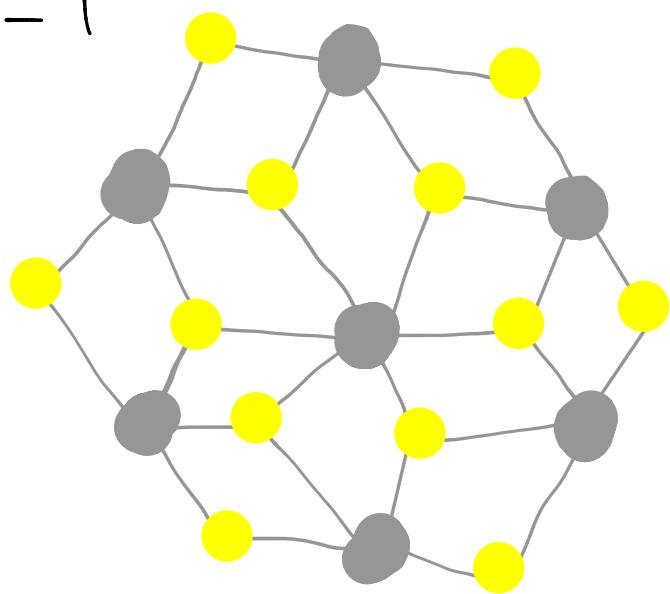
- a) Write down the expression for the (independent) electron wavefunction in the 1D solid.
- b) For this relatively simple case of one electron per unit cell, the allowed energies can be computed from the following formula

$$E(k) = \frac{\int_{-\infty}^{\infty} \psi^* H \psi dr}{\int_{-\infty}^{\infty} \psi^* \psi dr}$$

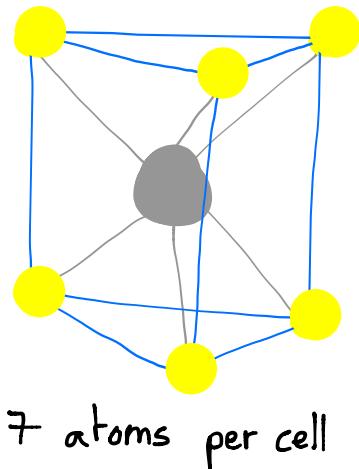
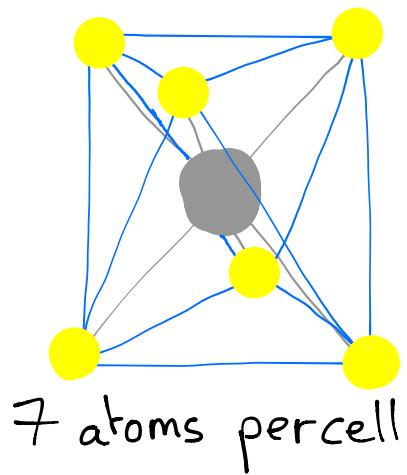
which is the expectation value of the electron energy which is also interpreted as the average energy. Determine the energy dispersion within the nearest neighbor formalism, and sketch the band structure.

2. Bravais lattice of TMDs:

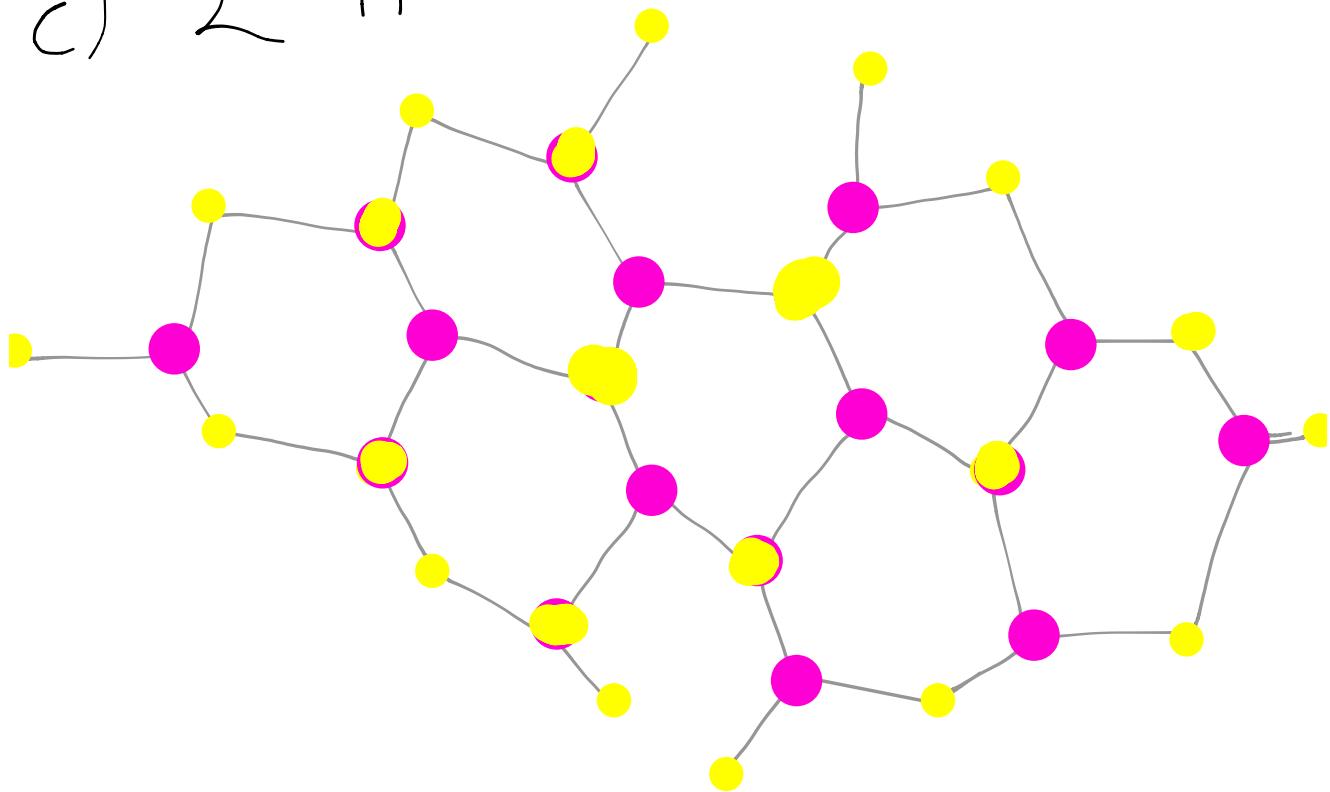
a) I-T



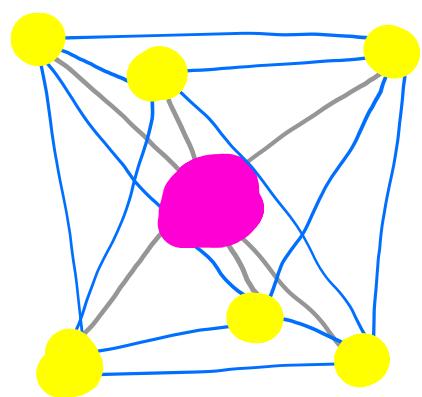
b) I-T



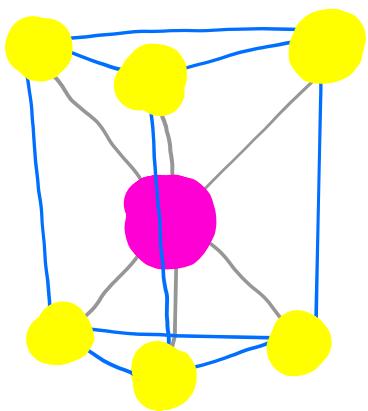
c) 2-H



d) 2-H



7 atoms per cell



7 atoms per cell

e) Examples of a TMD in:

i - 1T Structure \rightarrow ReS_2

ii - 2H Structure \rightarrow NbSe_2

iii - 3R Structure \rightarrow TaX_2

3. 1D Tight-binding model:

$$a) \Psi(x) = e^{ikx} u(x)$$

$$b) E(k) = \frac{\int_{-\infty}^{\infty} \psi^* H \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx}$$

$$\begin{aligned} ① & \int_{-\infty}^{\infty} e^{-ikx} u(x)^* H e^{ikx} u(x) dx & ② & \int_{-\infty}^{\infty} \psi^* \psi dx = 1 \\ & = \int_{-\infty}^{\infty} u(x)^* H u(x) dx & & \langle H \rangle_{u(x)} \\ & = E \int_{-\infty}^{\infty} u(x)^* u(x) dx & \boxed{E(k) = \frac{E}{1} = E} \\ & = E \end{aligned}$$

#4: A more accurate expression for the dispersion of electron waves in graphene (20 points)

- a) Show that for $S_{AB}(\mathbf{k}) \neq 0$, the energy dispersion is given by Eq. 3.38.
- b) Compare Eq. 3.37 to Eq. 3.38 by plotting both dispersions along the high-symmetry points Γ to K, and K to M, and quantify numerically the discrepancy between the two expressions at $\pm 1\text{eV}$. Take s_o to be 0.05.

Note that in general Eq. 3.38 is itself only an analytical approximation to the band structure computed via ab-initio methods (Figure 6), as such this exercise is meant in part to provide an awareness of the additional discrepancies introduced by the electron-hole approximation ($S_{AB}(\mathbf{k})=0$) particularly at energies substantially removed from the Fermi level.

#5: A long roadmap for 2D Materials (15 points)

A very long roadmap paper for 2D materials was recently published in nanoscale. This paper provides a global perspective for research and development of graphene and related 2D materials from the point of view of the \$1B EU graphene/2D flagship. You will find the paper interesting to read. Pace yourself since it is about 160 pages. The paper can be found here

<http://pubs.rsc.org/en/Content/ArticleLanding/2015/NR/C4NR01600A#!divAbstract>

Address the following questions.

- a) What is the most promising method of growing graphene for electronic applications? And explain the main advantage of that method. Also describe the current state of the art of that method.
- b) Which of the 2D materials (excluding graphene) offers the highest room temperature mobility? What is the corresponding bandgap of this material?
- c) Which of the 2D semiconductors (excluding graphene) offers the highest bandgap? What is the corresponding highest room temperature mobility of this material?
- d) What are the main advantages and challenges of graphene and 2D materials for the optoelectronics and photonics? List at least 2 advantages and challenges each.
- e) What are the main advantages and challenges of graphene and 2D materials for the health and environment? List at least 2 advantages and challenges each.

4. A more accurate expression for the dispersion of electron waves in graphene

a) For $S_{AB}(k) \neq 0$, E dispersion

$$E(k)^{\pm} = \frac{\pm \sqrt{1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y)}}{1 \mp 5\sqrt{1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y)}}$$

First, we have:

$$E(k)^{\pm} = \frac{E_0(k) + \sqrt{E_0(k)^2 - 4(S_{AA}(k)^2 - |S_{AB}(k)|^2)(H_{AA}(k)^2 - |H_{AB}(k)|^2)}}{2(S_{AA}(k)^2 - |S_{AB}(k)|^2)}$$

$$\text{where } E_0(k) = (2H_{AA}(k)S_{AA}(k) - S_{AB}(k)H_{AB}^*(k) - H_{AB}(k)S_{AB}^*(k))$$

Mathematically, electron-hole symmetry Forces $S_{AB}(k)=0$

$$\text{Therefore, } E(k)^{\pm} = \pm \sqrt{H_{AB}(k)H_{AB}^*(k)}$$

$$H_{AB}(k)H_{AB}^*(k) = 2(1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y))$$

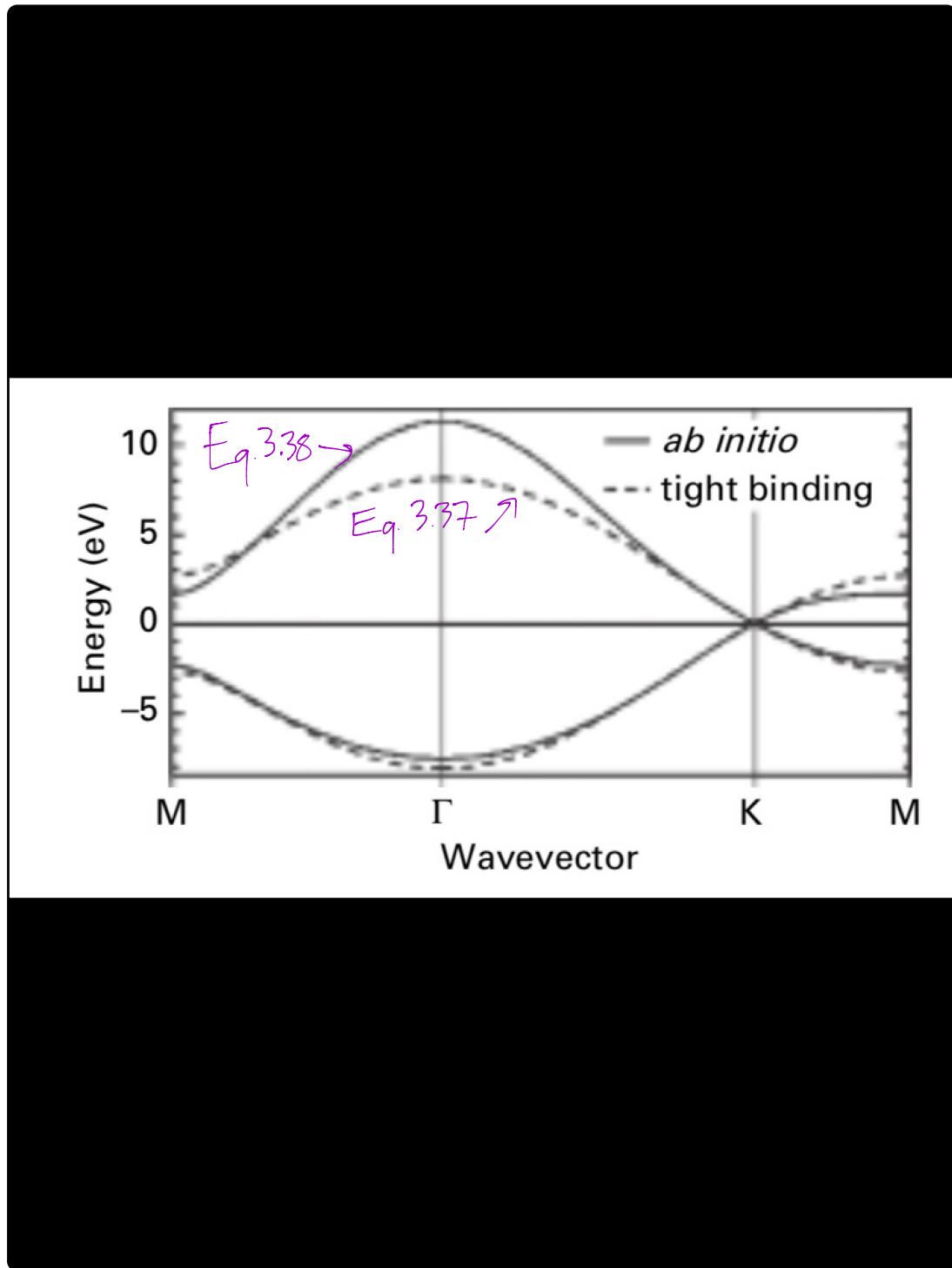
$$E(k)^{\pm} = \pm \sqrt{1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y)} \quad \text{Eq. 3.37}$$

This equation shows good agreement between NNTB and ab-initio computations at low energies.

However, a greater agreement at higher energies can be achieved by relaxing the e-h symmetry approximation, which leads to a non-zero $S_{AB}(k)$. For this case, the energy dispersion is:

$$E(k)^{\pm} = \frac{\pm \sqrt{1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y)}}{1 \mp 5\sqrt{1 + 4\cos(\frac{\sqrt{3}}{2}\alpha k_x)\cos(\frac{\alpha}{2}k_y) + 4\cos^2(\frac{\alpha}{2}k_y)}} \quad \text{Eq. 3.38}$$

b)



5. A long roadmap for 2D materials

- a) The most promising method for growing graphene for electronic applications is CVD (Chemical Vapor Deposition). The main advantage of CVD is that the quality of the resulting graphene is usually very high (high mobility). The current state of the art of this method is that it produces crystallites sizes of 50,000 μm at a sample size of 1000 mm. It is used to serve applications such as photonics, nanoelectronics, TCs, sensors, bio-applications, flexible electronics.
- b) Excluding graphene, phosphorene offers the highest RT mobility ($\mu \sim 286 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$). It has a bandgap of 0.9 eV.
- c) Excluding graphene, MoS₂ offers the highest bandgap (1.8eV). It has a RT mobility of $\sim 60\text{-}70 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$.
- d) **Optoelectronics and photonics:**
Advantages:
 - + High μ enables ultra-fast conversion of photons or plasmons to electrical currents or voltages.
 - + Graphene photonic devices can be fabricated using standard semiconductor technology.
Challenges:
 - Current polarization controlling devices are bulky and/or difficult to integrate for photonics.
 - For photo-detectors, we will need to increase responsivity, which might require a new structure, plasmonics and/or doping control.

e) Health & Environment:

Advantages:

+ It will offer the possibility to introduce more information on goods used on a daily basis, e.g. on food for safety and health, as well as on many other products.

+ Current research in nano-biosensors is experiencing a fast growth due to the wide range of novel applications for human healthcare.

Challenges:

-The GRM small size and unique physico-chemical properties may pose potential health and environment risks.

-Some GRMs have aerodynamic size that may lead to inhalation and deposition into the respiratory apparatus with implications on the formation of granulomas and lung fibrosis.