Simulating Band Bending of YbB_6 with Self-consistent Poisson-Scrödinger Method

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1 Introduction

YbB_6 is a topological insulator (TI) candidate which is now under quantum oscillation study in our group. According to previous ARPES results, it has a band gap around 100 meV and there's several surface Fermi pockets discovered. While it is likely that the surface states are topologically protected, it is also possible that it could be the surface states caused by surface band bending like in InN, which is not topologically protected. The main purpose of my work is to use simulation methods to find out whether it is possible to get surface band bending states under proper parameters.

2 Review of related works

Self-consistent Poisson-Schrödinger solution has been successfully applied to the system of InAs by Abe *et al.*, which used non-parabolic band structure derived from $\mathrm{k} \cdot \mathrm{p}$ approximation. The calculation method is iterative, starting from a trial potential and solve Poisson and Schrödinger equations repeatedly until some precision requirements are satisfied. This method can give both the surface bounded states and their dispersion relations, as well as the surface charge density.

Similar calculation was done on the system of InN by King *et al.* which used a different approach called modified Thomas-Fermi approximation. With this method, one only needs to solve the Poisson equation once to get the band bending picture, and then solve Schrödinger equation once to get the surface subbands. This can also give the dispersion relation of surface states.

My current work is based on the well-known Self-consistent Poisson-Schrödinger method originally designed to simulate semiconductors like Si or GaAs, which is implemented by Prof. G. Snider of University of Notre Dame. It can give the surface bounded states when the conduction band bends below the bulk chemical potential or the valence band bands above the bulk chemical potential, but cannot give the dispersion relation directly. (The method makes use of parabolic dispersion relation in carrier concentration calculations, so it is straightforward to get the dispersion relation manually.)

3 Method Overview

The main process of the algorithm is

1. Start with a trial potential $\phi(z)$;

2. Solve Schrödinger equation to get the wave functions:

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z) + q\phi(z)\psi(z) = E\psi(z)$$

3. Calculate carrier density from the wave functions;

4. Solve Poisson equation to get a new potential $\phi(z)$:

$$\frac{d^2}{dz^2}\phi(z) = -\frac{e[N_D^+ - N_A^- - n(z) + p(z)]}{\epsilon\epsilon_0}$$

with the boundary condition

$$\lim_{z\to\infty}\phi(z) = 0,\ \left.\frac{d\phi}{dz}\right|_{z=0} = \frac{eN_{SS}}{\epsilon\epsilon_0}$$

5. Iterate the steps above until precision requirement is satisfied.

4 Current Results

I applied the following parameters in the calculation:

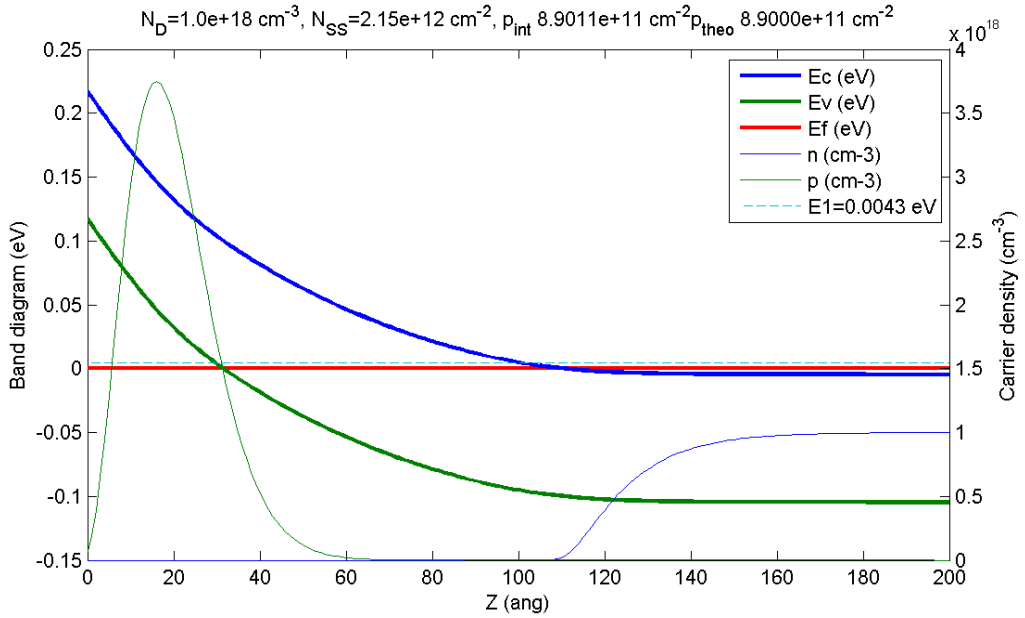
- Effective mass $m^* = 0.5m_e$;
- Rel. dielectric constant $\epsilon = 8.0$;
- Bulk band gap $E_g = 100\text{meV}$;
- Temperature $T = 5\text{K}$.
- Bulk electron density $n_b = 10^{18}, 10^{19}, 10^{20}\text{cm}^{-3}$.

The localized surface density N_{SS} scans from 10^{10}cm^{-2} to 10^{14}cm^{-2} in a geometric sequence for each bulk electron density n_b. After each calculation, if any hole bound states are found, integrate the hole density $p(z)$ to get the surface hole density p_{int}, and compare it with the theoretical values (based on the parabolic dispersion relation)

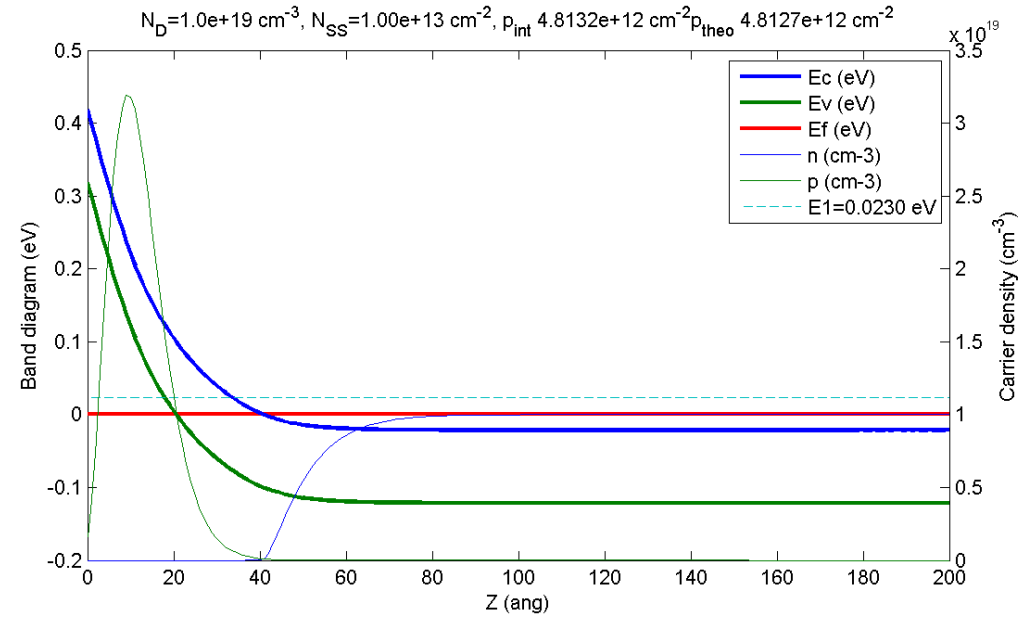
$$p_{\text{theo}} = \sum_k \frac{m^*}{\pi\hbar^2}(E_k - E_F).$$

The calculation results are summarized as follows.

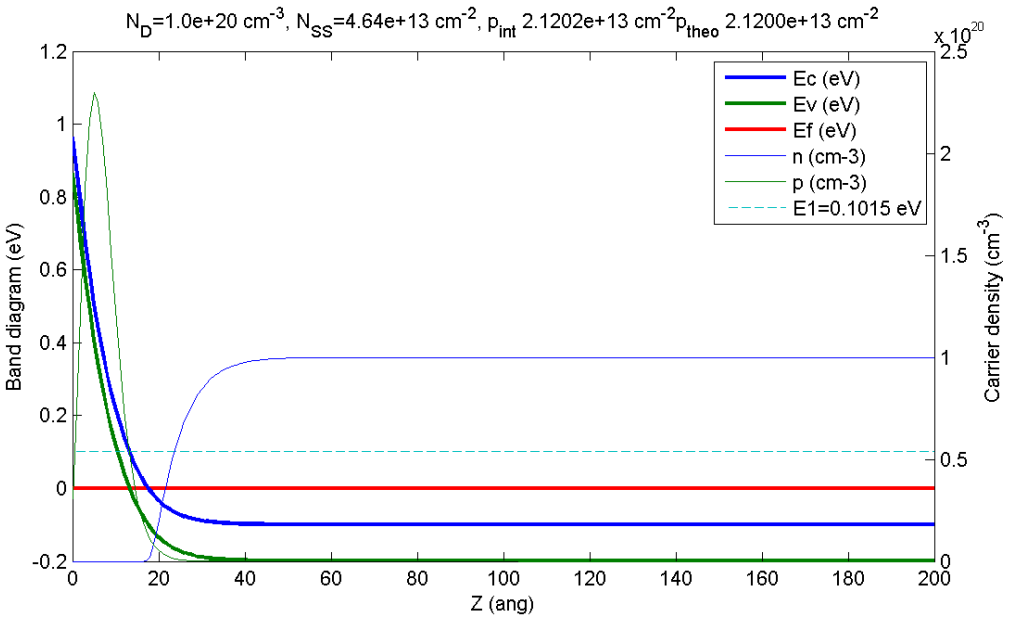
1. It is possible to get hole bound surface states above the Fermi level in the physical range of N_{SS}. In detail,
   - with $n_b = 10^{18}\text{cm}^{-3}$, first bound state occur around $N_{SS} = 2.15 \times 10^{12}\text{cm}^{-2}$;



- with $n_b = 10^{19}\mathrm{cm}^{-3}$, first bound state occur around $N_{SS} = 10^{13}\mathrm{cm}^{-2}$;

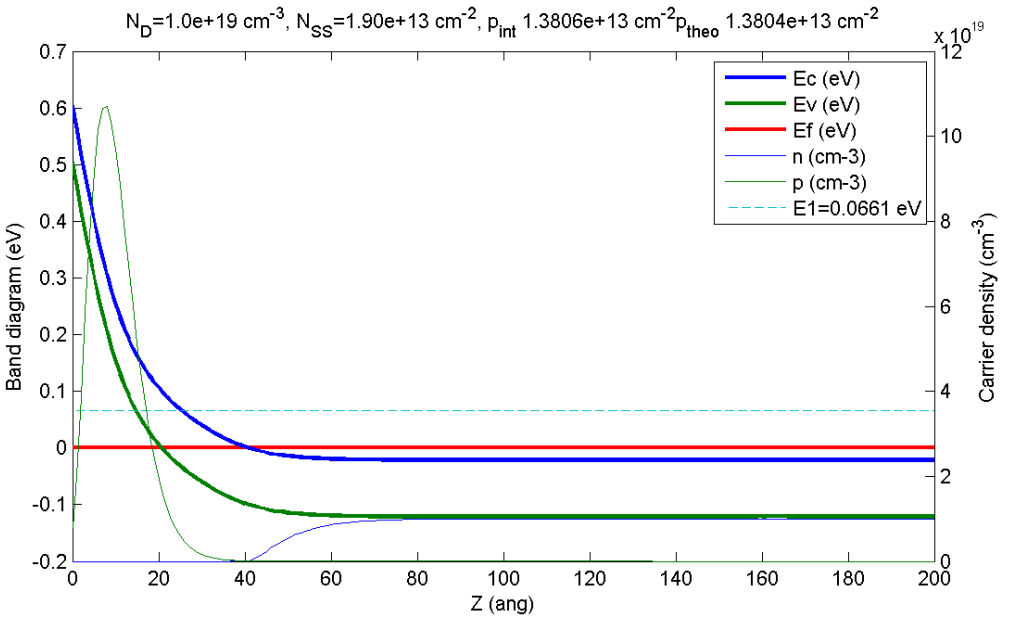


- with $n_b = 10^{20}\mathrm{cm}^{-3}$, first bound state occur around $N_{SS} = 4 \times 10^{13}\mathrm{cm}^{-2}$.

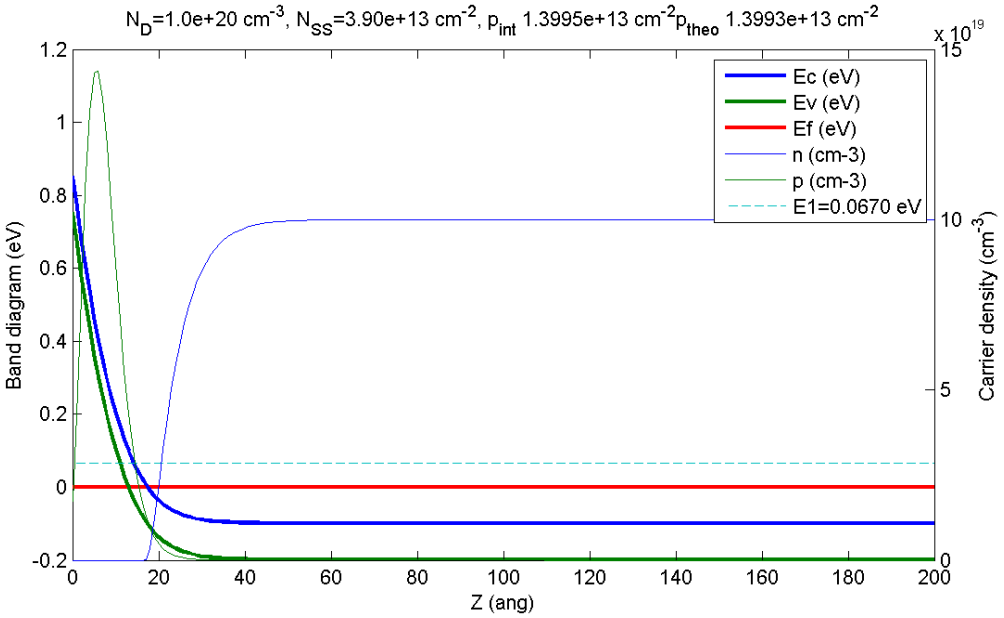


2. It is also possible to get hole surface state which gives surface charge density around the experiment value (with quantum oscillation 280T, the surface density is around $1.35 \times 10^{13}\mathrm{cm}^{-2}$):

   - with $n_b = 10^{19}\mathrm{cm}^{-3}$, we get the proper value with N_{SS} around $1.9 \times 10^{13}\mathrm{cm}^{-2}$;

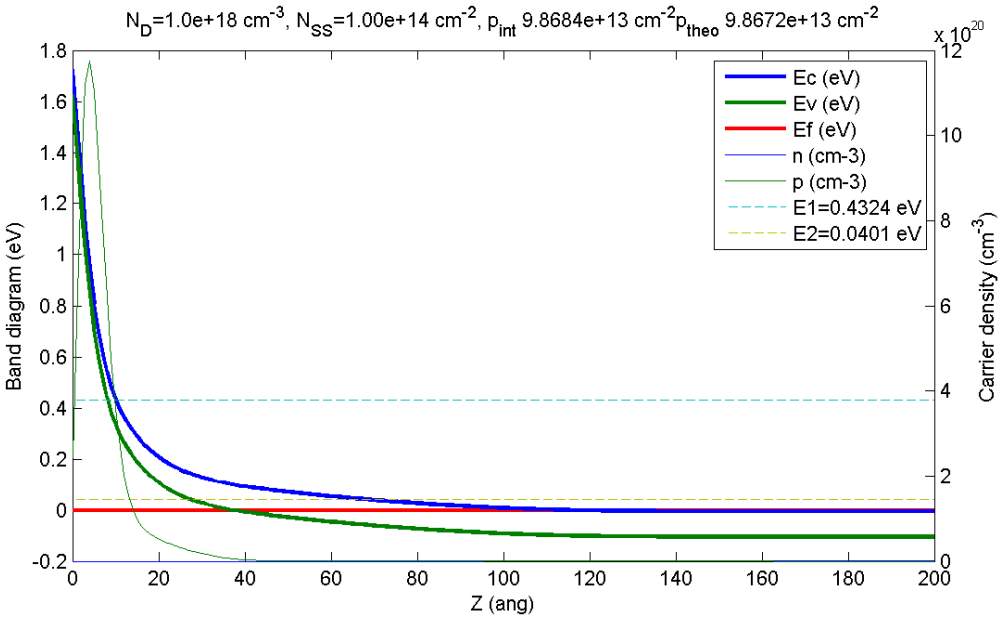


   - with $n_b = 10^{20}\mathrm{cm}^{-3}$, we get the proper value with N_{SS} around $3.9 \times 10^{13}\mathrm{cm}^{-2}$.

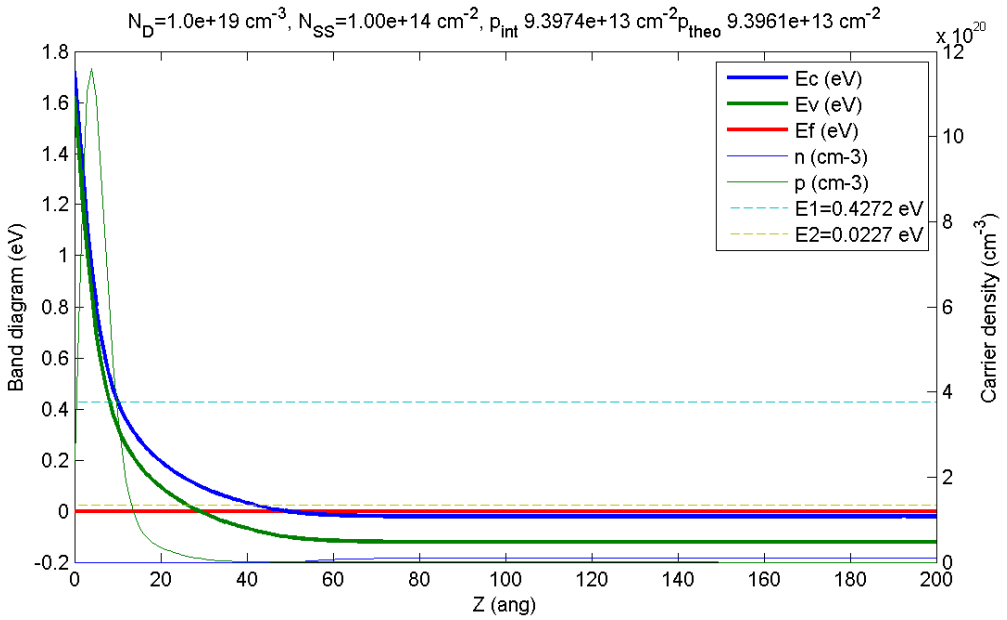


3. It is also possible to get two surface states with $N_{SS} \leq 10^{14}\mathrm{cm}^{-2}$, but the value is not so satisfying:

   - with $n_b = 10^{18}\mathrm{cm}^{-3}$, second bound state occur around $N_{SS} = 10^{14}\mathrm{cm}^{-2}$;



   - with $n_b = 10^{19}\mathrm{cm}^{-3}$, second bound state occur around $N_{SS} = 10^{14}\mathrm{cm}^{-2}$;



- with $n_b = 10^{20}\mathrm{cm}^{-3}$, second bound state cannot be found with $N_{SS} \leq 10^{14}\mathrm{cm}^{-2}$.

5 Next step

Although we have successfully obtained meaningful calculation results, there's still some problem. First, the program by Prof. Snider uses parabolic dispersion relation in the calculation, while in fact it might be non-parabolic like in the case of InN, which can make both the band diagram and the surface concentration calculation different. The slides provided by Jonathan also suggest such non-parabolicity. Second, the program cannot calculate bound hole states below E_F (or bound electron states above E_F) which can be found in the calculations of both InAs and InN.

In order to deal with the problems above, my intention is to borrow the idea of the InN calculation since its calculation method is simpler. I am now trying to repeat the work on InN by King *et al.*, and hopefully I can make some progress before the end of the program.

6 Acknowledgments

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References

[1] P. D. C. King, T. D. Veal, and C. F. McConville, *Phys. Rev. B* **77**, 125305 (2008).

[2] S. Abe, T. Inaoka, and M. Hasegawa, *Phys. Rev. B* **66**, 205309 (2002).

[3] I-H. Tan, G. L. Snider, L. D. Chang, and E. L. Hu, *J. Appl. Phys.* **68** (8), 4071 (1990).

[4] N. Xu *et al.*, arXiv:1405.0165 [cond-mat.str-el].

[5] M. Xia *et al.*, *Scientific Reports* **4**, 5999 (2014).