Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Christian Carbogno
Exercises: Dr. Christian Carbogno, Henrik Kowalski et al.

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http://www.itp.tu-berlin.de/menue/lehre/lv/ss_2017/pflichtveranstaltungen_masterstudium/theoretische_physik_vi_vertiefung_theoretische_festkoerperphysik_i_ii/

Theoretical Material Science: Exercise Sheet 6

Please hand in solutions by: Tuesday, June 6, start of the exercise class

Exercise 16 (10 points): *Electronic Structure of Semiconductors.*
One of the goals of electronic structure theory is the prediction, without any empirical parameter, of material properties. In the last exercise, we have tested the predictive power of density functional theory (DFT) in the local-density approximation (LDA) regarding the cohesive and bulk properties of real materials. Without a good prediction of cohesive properties, the calculation of the electronic structure of materials would not be possible. The objective of this exercise is to compute the electronic structure of three different important semiconductors (Si in its diamond phase, GaAs, and ZnSe). Starting from the bulk properties calculated in the last exercise, we will calculate the band structure and the density of states (DOS) in this exercise.

a) *Band structure and DOS of the diamond phase of Si.*
To complete this exercise, use the equilibrium lattice constant (a_0) found in the last exercise sheet. Use DFT-LDA and a 12×12×12 $\mathbf{k}$-point integration grid.

   (i) Calculate the band structure for the diamond phase of Si along the the high-symmetry path $L \to \Gamma \to X \to W \to K$.

   (ii) Calculate the DOS as a function of energy with respect to the Fermi level in the range of the valence bands.

   (iii) Plot the band structure and the DOS. Take a look at the DOS, can you identify the semiconductor behaviour? Looking at the band structure, identify the maximum of the valence band (VB) and the minimum of the conduction band (CB). What type of band gap (direct or indirect) is present? Compare the LDA predicted band gap with the experimental value of 1.17 eV. How is the prediction in comparison to experiment?

b) *Band structure and DOS of GaAs and ZnSe.*
GaAs is a III–V semiconducting compound (composed from elements of columns III and V in the periodic table) that crystallizes in the zincblende structure. The bonding character in the III–V semiconductors is predominantly covalent. On the other hand, ZnSe is a II–VI semiconductor (elements of colums II and VI). It also crystallizes in the zincblende structure. II–VI semiconductors present both ionic and covalent bonding character.
Use the equilibrium lattice constant (a_0) found for both materials in the last exercise and DFT-LDA to calculate the electronic properties of both materials. Consider an 12×12×12$\mathbf{k}$-point integration grid.

   (i) Calculate the band structure for GaAs and ZnSe along the high-symmetry path $L \to \Gamma \to X \to W \to K$.

   (ii) Calculate the DOS as a function of energy in the range of the valence bands for GaAs and ZnSe.

   (iii) Plot the band structure and the DOS for both compounds. Look at the band structures, identify the maximum of the VB and the minimum of the CB. What type of semiconductors are they? Compare the LDA predicted band gaps with the experimental values of 1.52 eV and 2.82 eV corresponding to GaAs and ZnSe respectively. Taking into account the diamond phase of Si, do you see any trend in the band gaps calculated with LDA?
   Comparing the band structures of both materials, how different are they from one another and from Si? What is the effect of the d electrons of Zn and Ga? Locate the minimum of the CB in both compounds (Γ point). What can you expect from the curvature of the band centered at the Γ point?

Please turn over!⟶

Exercise 17 (2 points): *Electronic Structure of Metals.*
The objective of this exercise is to show how drastically the atomic structure affects the properties, and to take a look at a metal.

Band structure and DOS of the fcc phase of Si. To complete this exercise, use the equilibrium lattice constant (a_0) found in the last exercise sheet. Use DFT-LDA and a $12\times12\times12$ $\mathbf{k}$-point integration grid.

(i) Calculate the band structure for the fcc phase of Si.
Choose the band structures along the high symmetry lines
$W \to L \to \Gamma \to X \to W$.

(ii) Calculate the DOS as a function of energy in the valence electron range.

(iii) Plot the band structure and the DOS. Do you identify the metallic behaviour from the band structure and the DOS? Take a look at the DOS, how should a free electron DOS look like? At energies where certain bands become flat, can you comment on the effect of "van Hove singularities" in the DOS?