Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Patrick Rinke, Dr. Alex Tkatchenko
Exercises: Dr. Volker Blum

June 6, 2012

http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/
wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/

Theoretical Material Science: Exercise Sheet 9

Please hand in solutions by: Wednesday, June 13, start of the exercise class

Exercise 21 (10 points): *Electronic structure in 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. Starting from the bulk properties calculated in the last exercise, we will calculate in this exercise, the bandstructure and the density of states (DOS) for Si in its diamond phase, GaAs, and ZnSe.

a) *Bandstructure 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 bandstructure for the diamond phase of Si.
Choose the bandstructures along the high symmetry lines
$L \to \Gamma \to X \to W \to K$.

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

b) *Bandstructure 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 8×8×8 $\mathbf{k}$-point integration grid.

(i) Calculate the bandstructure for GaAs and ZnSe.
Choose the bandstructures along the high symmetry lines
$L \to \Gamma \to X \to W \to K$.

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

(iii) Plot the bandstructure and the DOS for both compounds. Look at the bandstructures, identify the maximum of the VB and the minimum of the CB. What type of semiconductors are they? Compare the LDA predicted bandgaps 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 LDA calculated bandgaps?
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 22 (2 points): *Electronic structure in 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.

Bandstructure 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 12×12×12 $\mathbf{k}$-point integration grid.

(i) Calculate the bandstructure for the fcc phase of Si.
Choose the bandstructures 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 bandstructure and the DOS. Do you identify the metallic behaviour from the bandstructure 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?

- **Webpage of the lecture:**
http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
http://th.fhi-berlin.mpg.de/sitesub/lectures/spring_2012/
- **Lecture:** Tue. & Wed., 10:00 h -12:00 h (sharp!) in room EW 203, TU Berlin
- **Exercise:** Wed., 14:00 h in room EW 229
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids, Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festkörpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
  - Kohanoff: Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge University Press, Cambridge, 2006
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
  - Active participation in computational exercises
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler, Dr. Alex Tkatchenko, Dr. Patrick Rinke: by appointment
  - Dr. Volker Blum: Available Wed. 16:00 (after the exercise class) or by appointment