

Theoretical Material Science: Exercise Sheet 5

Please hand in solutions by: **Wednesday, May 16**, start of the exercise class

Exercise 12 (4 points): *Close-packed structures*

- What is the packing density achieved by the bcc- and fcc-structure, respectively?
- Show that a close-packed structure with ABC stacking is identical to the fcc-structure.

Exercise 13 (4 points): *Pointgroup O_h and that of diamond*

The full octrahedral group O_h contains the following symmetry elements: E , $6C_4$, $8C_3$, $(6+3)C_2$, $3\sigma_h$, $6\sigma_d$, i , $6S_4$ and $8S_6$. Determine the matrix representation for each of the following point transformations contained in the O_h group:

- Rotations C_3 (rotation angle $\frac{2\pi}{3}$ about the cube diagonals, e.g. $(1, 1, 1)$ -axis,
- The three rotations C_2 (rotation angle π) about the X , Y , Z axes,
- Reflections σ in the plane perpendicular to $\mathbf{n} = (-1, 1, 0)$ through the origin,
- Inversion,

- with respect to the standard basis of \mathbf{R}^3 ;
- with respect to the basis vectors \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 of the fcc lattice (primitive cell).
- Show that while the inversion i is not a symmetry transformation of the diamond structure, C_3 , C_2 and σ are (The pointgroup of diamond is the tetrahedral group T_d).

Note: Diamond has an fcc-lattice. The two-atom basis of the crystal is given by a C-atom at position $\mathbf{s}_1 = (0, 0, 0)$ and a C-atom at position $\mathbf{s}_2 = \frac{a}{4}(1, 1, 1)$, with a being the lattice constant.

Exercise 14 (4 points): *Brillouin zone integrals*

This task is a computational exercise that illustrates the importance of accurate Brillouin zone sampling in practice. As before, the below questions are just a "skeleton" – please refer to the accompanying, more detailed script for more information. In periodic solids, Bloch's theorem tells us that a good quantum number to count "states" is the crystal momentum \mathbf{k} , whose unique values are confined to the first Brillouin zone. For integrated quantities, this means that the usual sums over states i are replaced by an integral over all \mathbf{k} and different states n that correspond to the same \mathbf{k} :

$$\sum_i [\dots] \rightarrow \sum_n \int_{\mathbf{k} \text{ in 1. BZ}} d^3k [\dots]$$

For any quantity that is an average over states—for example, the total energy or the electron density—the k -space integral must be carried out explicitly, and with sufficient accuracy. Investigate the influence of a finite \mathbf{k} -space integration grid for Si:

- For the diamond phase of Si, at the experimental lattice parameter $a=5.43 \text{ \AA}$, and using density-functional theory in the local-density approximation, calculate and plot the convergence of the cohesive energy with the integration quality of the Brillouin zone. How many integration points are needed for good convergence (few meV)? Is the convergence of the total energy variational with integration quality?
- For a given \mathbf{k} -space integration grid, plot (i) the three-dimensional electron density $n(\mathbf{r})$ and (ii) the electron density *difference* to a simple superposition of free atom densities. What is the predominant density change compared to simple free atoms, and does it match your physical intuition?
- For each \mathbf{k} grid, the code gives you an estimate of the highest occupied state, the lowest unoccupied state, and their difference—the equivalent of the "band gap," but computed in Kohn-Sham theory. Is this "Kohn-Sham band gap" large enough compared to experiment? How does it evolve with improving integration quality of the Brillouin zone? What can you learn from the (approximate) location of the lowest unoccupied state in \mathbf{k} -space?

Please turn over! →

- **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