Technische Universität Berlin
Institut für Theoretische Physik
Prof. Dr. Matthias Scheffler
Dr. Volker Blum, Dr. Clive Emary
Dipl. Phys. Philipp Zedler

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http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/

Theoretical Material Science: exercise sheet 8

Return: Monday, June 16 in the exercise

Exercise 19 (4 points): *Lattice sums*
We define the lattice sum $A_n^{crystal}$ for a crystal structure as

$$A_n^{crystal} = \sum_{I \in crystal} \alpha_I^{-n},$$

where the dimensionless quantity α_I is the proportionality constant between the position $\mathbf{R}_I$ of atom I in the crystal and the nearest neighbour distance c:

$$|\mathbf{R}_I| = \alpha_I c.$$

Compute the lattice sums A_6 and A_{12} up to third nearest neighbours in the fcc, the bcc, and the sc structure, and compare with the converged values in the literature. Why are A_6 and A_{12} relevant quantities for the stability of a noble gas crystal?

Exercise 20 (8 points): *Plot the electron density for Si, Ge, GaAs and ZnSe*
Use the Hamiltonian from the band-structure exercise and obtain the corresponding wavefunction for the four materials in Table 1. Plot the valence electron density $n(\mathbf{r}) = \sum_{\mathbf{k}} \sum_n^{VB} |\varphi_{n,\mathbf{k}}(\mathbf{r})|^2 \approx \sum_{\mathbf{n}}^{\mathbf{VB}} |\varphi_{\mathbf{n},\mathbf{k}}(\mathbf{r})|^2$ for,

a) The Γ point (a bad choice for representing the $\mathbf{k}$ summation), and

b) the special $\mathbf{k}$ point $\frac{2\pi}{a}(0.6223, 0.2953, 0)$ (a good choice for representing the $\mathbf{k}$ summation over the full Brillouin zone).

Discuss the trend of the special $\mathbf{k}$-point result for Si→Ge→GaAs→ZnSe in terms of the nature of the chemical bond of the materials. Hint: Use spherical cutoff for the basis states in the Hamiltonian matrix, $(\mathbf{G}+\mathbf{k})^2 \leq (\frac{2\pi}{a})^2 21$. Use ContourPlot to plot the electron density for the (110) plane. Figure 1 shows the (110) cut through the diamond crystal and the zigzag chain of atoms in that plane.

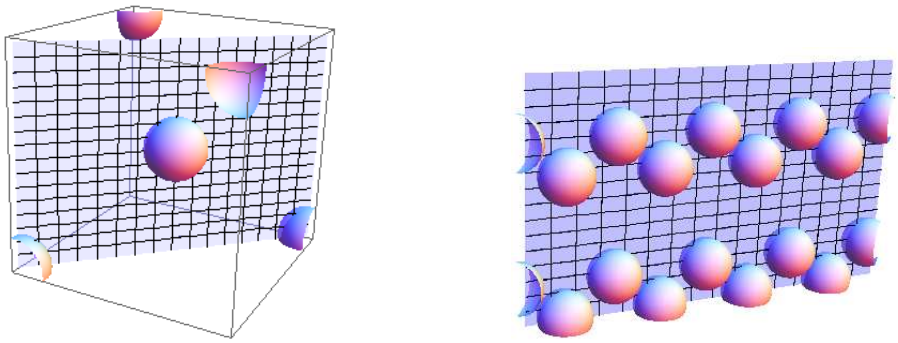

Figure 1: (Left): Unitary cube of the diamond crystal showing the (110) plane. (Right): Illustration of the characteristic zigzag pattern formed at the (110) plane.

	a [Å]	V_0^S	V_3^S	V_4^S	V_8^S	V_{11}^S	V_0^A	V_3^A	V_4^A	V_8^A	V_{11}^A
Si	5.43	0.00	-0.21	0.00	0.04	0.08	0.00	0.00	0.00	0.00	0.00
Ge	5.66	0.00	-0.23	0.00	0.01	0.06	0.00	0.00	0.00	0.00	0.00
GaAs	5.64	0.00	-0.23	0.00	0.01	0.06	0.00	0.07	0.05	0.00	0.01
ZnSe	5.65	0.00	-0.23	0.00	0.01	0.06	0.00	0.18	0.12	0.00	0.03

Table 1: Lattice constants and pseudopotential form factors for four materials of the diamond or zinc-blende structure given in Rydberg units.

Please turn over!⟶

- **Webpage of the lecture:** http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/
- **Lecture:** Tue. & Fri., 10:00 a.m.-12:00 p.m. in room EW 203, TU Berlin
- **Exercise:** Mon., 14:00 a.m. in room H 1029
- **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: Festk?rpertheorie, 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
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler: on appointment
  - Dr. Volker Blum: on appointment
  - Philipp Zedler: Wed, 11:00 - 12:00 a.m. in room EW 711