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 6

Return: Monday, June 2 in the exercise

Exercise 15 (12 points): *Electronic band-structure calculations with pseudopotentials*
The electronic Hamiltonian of a crystal has the form:

$$H = -\frac{\hbar^2}{2m}\nabla^2 + v^{eff}(\overrightarrow{r})i \quad . \tag{1}$$

The pseudopotential $v^{eff}(\overrightarrow{r})$ can be expanded in reciprocal lattice vectors $\mathbf{G}$:

$$v^{eff}(\overrightarrow{r}) = \sum_{|\mathbf{G}|\leq G_0} \left(S^S(\mathbf{G})V^S_{\mathbf{G}} + \imath S^A(\mathbf{G})V^A_{\mathbf{G}}\right)\exp^{-\imath\mathbf{G}\overrightarrow{r}} \quad . \tag{2}$$

For crystals of the diamond or zinc-blende type with a cubic unit cell and fcc structure with 2 basis atoms at positions $\mathbf{r}_1 = a(\frac{1}{8},\frac{1}{8},\frac{1}{8}) \equiv \tau$, and $\mathbf{r}_2 = -\tau$, the structure factors S have the form:

$$S^S(\mathbf{G}) = \cos(\mathbf{G}\tau), \quad S^A(\mathbf{G}) = \sin(\mathbf{G}\tau) \quad . \tag{3}$$

Represent the Hamiltonian in the basis of plane waves with wave vectors $\mathbf{G}+\mathbf{k}$ with suitable reciprocal lattice vectors $\mathbf{G}$ and wave vectors $\mathbf{k}$ from the first Brillouin zone. The cubic constants a and pseudopotential form factors $V^{S/A}_{\mathbf{G}}$ in dependence of $|\mathbf{G}|$ are given in Table 1 for four different materials. Calculate the electronic band structure from the resulting eigenvalue equation of the Hamiltonian matrix for $\mathbf{k}$ going between high-symmetry points $L \to \Gamma \to X$ in piecewise linear paths.
Hint: Use Rydberg atomic units and choose the cutoff $G_0^2 = 11(\frac{2\pi}{a})^2$ for the plane-wave expansion. Then plot the resulting band structures in units of eV and choose the zero energy offset (separation of valence and conduction bands) at the value of the second band at the Γ k-point.

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

	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

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