MATERIALS PHYSICS II   FALL 2007   HOMEWORK PROBLEMS 2

Return to Robert (mailbox Physics 2nd floor) by Tuesday 25.9.2007 at noon

1. Derive the dispersion relation $\epsilon(\mathbf{k})$ for fcc and bcc lattices in the tight-binding approximation, assuming one s-electron per lattice site and only the nearest-neighbour interactions. Evaluate the bandwidth in each case and relate it to the coordination number.

2. (a) Consider a 2-dimensional square lattice with lattice constant a and take

$$U(\mathbf{r}) = -4U_0 cos\frac{2\pi x}{a} cos\frac{2\pi y}{a}.$$

Calculate the Fourier transform

$$U_{\mathbf{q}} = \int_{unitcell} \frac{d\mathbf{r}}{\Omega} e^{-i\mathbf{q}\cdot\mathbf{r}} U(\mathbf{r}).$$

(b) For $\mathbf{k}_1 = (\pi/a, \pi/a)$, $\Psi(\mathbf{k}_1)$ will couple strongly to three other components: $\Psi(\mathbf{k}_2)$, $\Psi(\mathbf{k}_3)$, $\Psi(\mathbf{k}_4)$. What are these vectors and why (identify the corresponding reciprocal lattice vectors $\mathbf{K}$)? (c) Evaluate $U_{\mathbf{K}}$ for those vectors. Show that $U_{\mathbf{K}} = U_{-\mathbf{K}}$. Therefore, perturbation theory can be reduced to a subspace involving only two components, say, $\Psi(\mathbf{k}_1)$ and $\Psi(\mathbf{k}_2)$. (d) Write down Schrödinger's equation in this subspace and solve the resulting 2x2 system of equations and find the two allowed energies at Bloch index $\mathbf{k}_1$. (e) Sketch $\varepsilon_{\mathbf{k}}$ for the lowest two bands along the line $\Gamma - T$ ($T = (\frac{\pi}{a}, \frac{\pi}{a})$) and indicate the size of the energy gap at T.

3. *Quasi-2D electron gas.* (a) Consider a free-electron gas in an external potential, for which $V = 0$ for $|z| < d/2$ and $V = V_0$ for $|z| > d/2$. What is the (energy) density of states for $V_0 \to \infty$? (b) Assume that $d = 100$ Å. Up to what temperatures can we consider the electron gas to be two-dimensional? If one can produce a potential of $V_0 = 100$ meV and reach a temperature of 20 mK, what is the range of thicknesses feasible for such a two-dimensional system? (This kind of quasi-2D electron gas is found in semiconductor devices and is used for investigations of, e.g., quantum Hall effect.)

4. *Quasi-1D metal.* In a quasi-1D metal, the overlap of partially occupied electronic states (orbitals) is large along one direction, but much smaller in the other two directions (one realization is the so-called KCP metal, Elliott fig. 8.15, attached on the 3rd page). Assume an electron band of the form

$$E_{\mathbf{k}} = \frac{-E_0}{2}[Acos(k_x a) + Bcos(k_y b) + Bcos(k_z b)]$$

where k_x, k_y, k_z are the components of the electron momentum and $A >> B$. How will the constant-energy cuts look on the (k_x, k_y) plane? Show that for a nearly half-filled band the density of states (and therefore all the thermodynamic properties!) of this system is similar to a truly one-dimensional electron gas. (Hint: use $D(E) = 2\int(2\pi)^{-d}| \bigtriangledown_{\mathbf{k}} E_{\mathbf{k}}|^{-1}dS$)

5. Examine the computed band structures for copper, silver and gold, attached on the last page (this data is taken from a German PhD thesis written by Dr. Ingo Opahle, Dresden 2001). Each figure shows the same result calculated with two variants of theory. Do not pay attention to these details, it is the general structure of the bands which is more important. On the basis of these figures, explain why copper and gold metals have colour (orange-yellow), but silver metal is colourless (grayish)! Explore literature if needed. Even Google might be able to help you. Whatever is your explanation, to get full points you need to connect the physics somehow to the shown band structure curves!

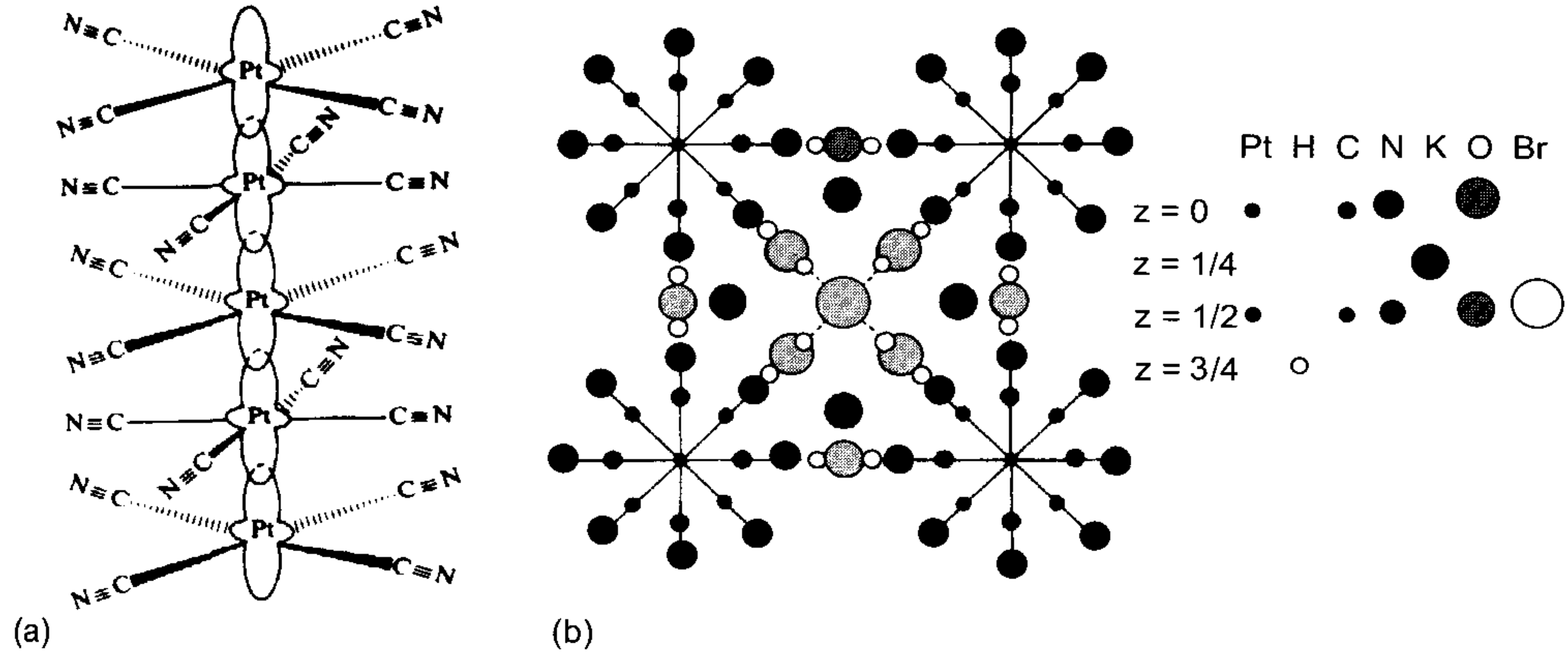
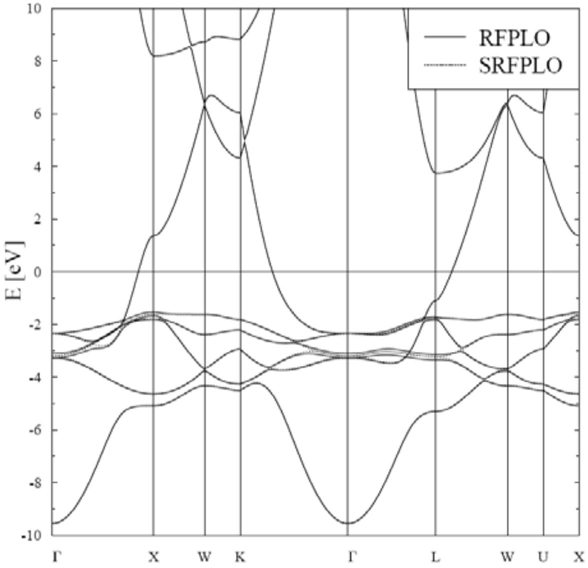
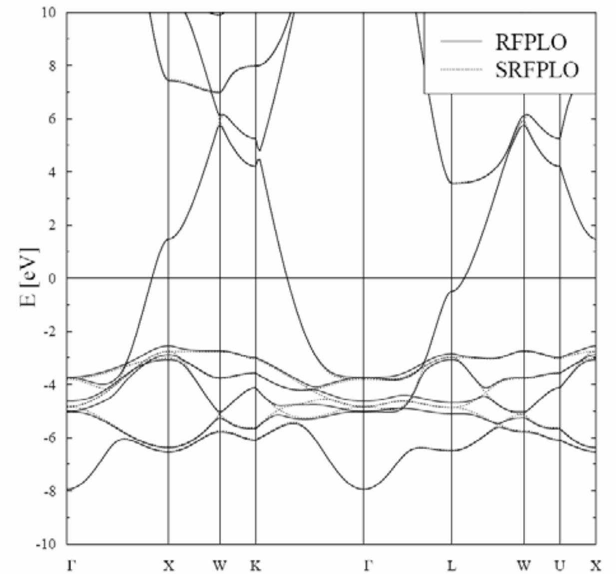


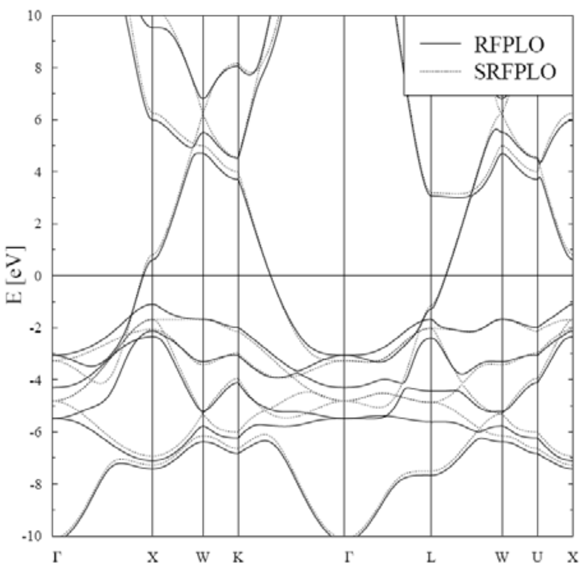
Fig. 8.15 Structure of the 1D metal, KCP ($K_2Pt(CN)_4Br_{0.3}.3H_2O$), consisting of a stack square-planar $Pt(CN)_4^{2-}$ clusters with Pt–Pt bonding, via overlap of $5d_{z^2}$ orbitals, along the chai (a) side view; (Cox (1987). *Electronic Structure and Chemistry of Solids*, by permission of Oxfo University Press) (b) projection. (Smart and Moore (1992). *Solid State Chemistry*, Fig. 4.7: wi kind permission from Kluwer Academic Publishers)



copper



silver



gold

From: Ingo Opahle, PhD Thesis
Dresden 2001