Exercises Functional Materials

1) Name four types of chemical bonding for solid state compounds with examples!

2) Define the terms “phase” and “polymorphism”!

3) Name differences between a real crystal and an ideal crystal!

4) What do you understand under phase transition 1^{st} or 2^{nd} order?

5) What do you understand under formation of mixed crystals? Which requirement is necessary that two elements or solid compounds form a complete solid solution?

6) How could you define the terms intercalation mixed crystal and substitutional mixed crystal?

7) Please list the defects according to their geometric appearance and name an example for each defect!

8) Please mention the effect on material properties for three different defect types and give examples!

9) A sample of doped silicon, which is used for the preparation of semiconductors contains 10^{21} Al atoms per m^3. Please calculate the mass fraction from aluminium of such a silicon sample!

10) A solid state has a band gap of 3.0 eV. Which colour do you expect for this material?

11) There should be prepared a red pigment on basis of an undoped solid state. Which band gap should have this substance?

12) In which range is the Hook´s law valid?

13) Please explain the increasing of defects in a material if the temperature increase!

14) What do you understand under the term “colour centre”? Please name some physical methods to characterise these defects.

15) The mineral grossular $Ca_3Al_2[Si_3O_{12}]$ has garnet structure. In which way one could derive the yttrium-aluminium-garnet (YAG) and yttrium-iron-garnet (YIG) composition from grossular?

16) What do you understand under a solid solution? Please mention two examples which are important in technical applications!

17) Please name two examples for each magnetic, optic, and superconductive materials!

18) Please explain the terms “isotropy” and “anisotropy”!

19) Which hardness tests do you know? For which class of material are they used?

20) 50 g Nb will be up heated by 75 °C. Calculate the specific heat capacity and the amount of heat which is added from the molar heat capacity.

21) Please calculate the amount of heat to warm up 1 kg of each of the following substances for 50 K.

    a. Lead

    b. Nickel

    c. Si_3N_4

    d. Nylon-6,6

22) The surface of the lake Zurich amounts to A = 67.2 km^2. The volume is about V = 3305*10^6 m^3 (volume-expansion coefficient of H_2O γ = 207*10^{-6} K^{-1}).

    a. How much increases the water surface by an increase of the temperature of 5 °C? (Assumption: no enlargement of the water surface by increasing of the water surface.)

    b. Why is such an increase of the water surface during the summer term not observed?

23) Assumption: The “Deutsche Bahn” used one cord of steel for 290 km tracks between Berlin and Hamburg. To what length would have expanded the track between the coldest winter day (-20 °C) and the warmest summer day (34 °C)? The linear thermal extension coefficient is α_{steel} = 1.2*10^{-5} K^{-1}.

24) Please name typical characteristics of semiconductors and of some semiconductor materials.

25) What do you understand under an intrinsic and doped semi-conductor?

26) Which processes are used for the dopant of semi-conductors? Describe one process.

27) How are metal, semi-conductor and insulator distinguished in the band model? Sketch the different dispositions of bands. Which statement could be true for the position of electrons?

28) In which way depends the intrinsic concentration of charge carrier n_i from the temperature and the band gap?

29) Please sketch the concentration of charge carrier n of a doped semi-conductor as a function of temperature in an Arrhenius-plot (ln(n) over 1/T).

30) Please calculate the covalent part for the following ionic compounds.

    a. AlF_3

    b. Al_2O_3

c. AlN

d. GaN

31) Please define the following terms.

a. Intrinsic semi-conductor

b. Impurity semi-conductor

c. Defect semi-conductor

32) What influence the conductivity of the semi-conductor material in the following components?

a. Solar cell

b. Thermistors

c. Field-effect transistor

d. Photoresistor (light-dependent resistor LDR)

33) The M^{2+} Ionics belay at octahedral gaps in pyritic sulphides of transition metals. Two bands emerge by the formation of the d-band. Can you deduce from the following properties of different sulphides

a. If the d-electrons are located or delocalised.

b. In which band will the d-electrons move, if the electrons are delocalised.

c. Between which bands could the band gap belay (in semi-conductors).

- MnS_2: anti-ferromagnetic (T_N=78K), insulator, paramagnetism of five unpaired electrons above T_N
- FeS_2: diamagnetic, semi-conductor
- CoS_2: ferromagnetic (T_C=115 K), metallic conductor

34) Estimate the number of free charge carrier for Ge at room temperature (σ = 0.02 $\Omega^{-1}cm^{-1}$, μ_e = 3800 $cm^2/V*s$, μ_h = 1820 $cm^2/V*s$, q = $1.602*10^{-19}$ As). Ge crystallises in a cubic diamond structure with a = $5.6575*10^{-8}$ cm and Z = 8 (atom/unit cell). Who much is the part of excited electrons in the valence band?

35) Please calculate the necessary number of charge carrier to get a p-conductive Si with a conductivity of 100 $\Omega^{-1}cm^{-1}$.

36) At which temperature do you have to cool down cobalt so that the electric conductivity is twice as big as at room temperature?

37) How can you ascertain, if the substances are a metal or a semi-conductor?

38) Please calculate the electric conductivity from nickel by -50 and 500°C.

39) What effects p-dopant and n-dopant in a semiconductor? Which species can you use as dopants for Si?

40) The efficiency of a silicon solar-cell decreases with increasing temperature.
    a. Who could you explain this?
    b. There is an area of solar cells at the Sahara. Which thickness of solar cells should be useful to achieve a high efficiency? A thick or thin one?

41) Name five compound semiconductors and order these by increasing band gap. How does the colour change by increasing band gap?

42) Name two defect semi-conductor each with p- and n-conduction.

43) La_2CuO_4 will be superconductive, if the middle oxidation state of the cooper is +2.2. How much Sr^{2+} and Ba^{2+} is necessary to get these oxidation state of cooper? Please name the molecular formula.

44) Why can`t a good conductor pass into a superconductive state? Please explain it.

45) The compound $Y_2Br_2C_2$ is two-dimensional metallic conducting and a superconductor with a transition temperature of about 5 K.
    a. Explain the metallic properties by the help of MO-diagram.
    b. Which bond order exists at the C_2-unit?
    c. What kind of structural exception can be concluded because of the above-mentioned properties?

46) Please explain the term “cooper pair”.

47) What is meant by fermion or bosons? Name two example for each term.

48) Which properties characterise structure types which are used in dielectric materials?

49) Please calculate the polarisation od cooper atoms, when the electrons of the cooper atom are shifted relative to the core of the atom by 0.1 nm because of an electric field.

50) How could you produce a space saving condenser with a capacity of e.g. 1 µF?

51) What types of condenser do you know?

52) Name two chemical compounds, which show a high permittivity and give an explanation.

53) The Curie-temperature and the permittivity change in ferroelectrics with hydrogen bridge bond, when hydrogen is substituted to deuterium. What conclusion could be drawn caused in the electric properties of this compound?

54) There is a plate capacitor with only two plates and a micaceous layer (ε=7) with a thickness of 0.000254 cm, used as a dielectric material. How big should have been the plates to get a capacity of 0.0252 µF? How could you effective decrease the plate size?

55) Which type of magnetism can occur in atoms, molecules or ionic solids?

56) Name three diamagnetic and three paramagnetic diatomic molecules. Explain your choice.

57) How can you determine, if a substance is diamagnetic or paramagnetic?

58) Calculate the theoretical magnetic moment ($\mu_{mag.}$ in [μ_B]) for the octahedron high-spin-complex $[Fe(ox)_3]^{3-}$ {Trioxalatferrate(III)} and the low-spin-complexes $[Fe(CN)_6]^{3-}$ {Hexacyanoferrate(III)} and $[Fe(CN)_6]^{4-}$ {Hexacyanoferrate(II)} by the help of the "spin-only-formula".

59) The nickel-complex $[Ni(PPh_3)_2Cl_2]$ is paramagnetic, whereas the analogical palladium-complex is diamagnetic. Propose an explanation for this finding based on the electron configuration.

60) $ZnFe_2O_4$ is an inverse spinel at low temperature. Which type of magnetism could you expect in this state?

61) Sketch the trend of magnetic susceptibly as a function of the temperature for the following magnetic materials.

    a. Diamagnet

    b. Paramagnet

    c. Antiferromagnet

    d. Ferromagnet

62) In which organic molecules do you expect paramagnetic behaviour?

63) Determine the saturation magnetization and the resultant magnetic field for iron. Assumption: Each iron atom has a magnetic moment of 1 Bohr magneton (1 μ_B) (density: ρ = 7900 kg/m^3).

64) The magnetic moment of the complexes $[Mn(H_2O)_6]^{2+}$, $[Fe(H_2O)_6]^{3+}$, $[MnCl_4]^{2-}$ and $[FeCl_4]^{2-}$ are 5.92 μ_B for each. What could tell you this finding about the geometric and electronic structure of these complexes?

65) The magnetic moment of $CrCl_3$ is 3.81 μ_B. How much unpaired electron have this compound?

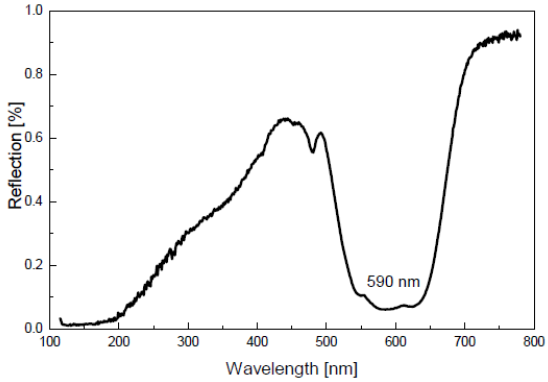
66) How can ferromagnetic properties emerge? Please explain this. In which compounds do you expect ferrimagnetism?

67) Which type of magnetism do you expect for binuclear, μ_2-oxoverbrückte Mn^{2+}-complexes?

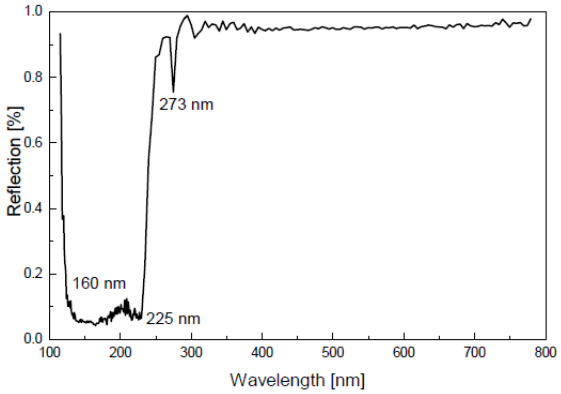
68) The garnet $Sm_{0.4}Y_{2.6}Ga_{1.2}Fe_{3.8}O_{12}$ is used as a storage material in magnetic bubble storages. Explain the emergence of ferromagnetic properties because of the orientation from the spin vectors for the different ionics.

69) Please refer electronic transition to the absorption bands you can see in the following reflection spectra.

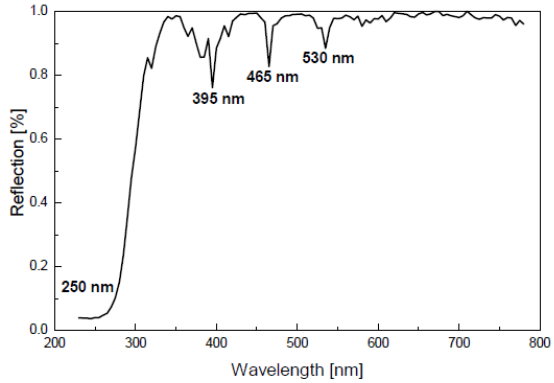
a. $CoAl_2O_4$



b. Gd_2O_3



c. Eu_2O_3



70) Explain the reason of colourfulness from blue cooper(II) sulphate (blue vitriol) solution.

71) Explain the following observations:

a. Complexes will disintegrate in sunlight, if they exhibit charge-transfer bands in visible range.

b. Complexes will be often strong coloured, if they present two metals in nearest vicinity and different oxidations state.

c. Complexes of trivalent europium are often without colour but (weak) yellow coloured with strong π-donor-ligand.

72) What is based on the usage of a smalt (cobalt glass) at the observation of characteristic flames from potassium?

73) Calculate the part of specular reflected radiation for lead glass (n = 2.50) and quartz (n = 1.55) for a wavelength of 589 nm at perpendicular incidence

74) How could light efficient decelerated?

75) Order the following white substances to increasing band gap or refraction index.

TiO_2, SiO_2, Al_2O_3, Y_2O_3, Lu_2O_3

76) Determine the critical band gap of complete transmittance or the absorption of visible light.

77) Propose a surface coating for a conception of a radar hidden plane.

78) The decay time of luminescence is about $\tau_{1/e}$ = 3.5 ms for the red PDP-luminescent substance (Y,Gd)BO_3:Eu. How long does it take, before the intensity decays to 1% of the intensity at beginning after pumping? Which relative intensity would have a red pixel with a display refresh rate from 100 Hz in the off state, if it was in the last picture in the on state?

79) Which technical measures can influence the refraction index of glass?

80) Which method could be used to increase the decoupling of light from a light producing solid (LED, OLED)?

81) Sketch a reflection spectrum for a material with a band gap of 2.5 eV in the range between 300 and 800 nm, there are no other absorption centre. Assumption: The band gap is defined as the point with the main change of absorption coefficient, the inflection point.

82) How could you dope a YAG crystal to obtain a solid-LASER with an emission in the UV-B, in the red or in the infrared spectral range?

83) A variety of extrasolar planets would have been discovered in the last few years. Which optical measuring procedure could detect live on these planets?

84) Which morphological requirement should be fulfilled from a catalytic pigment? Which form have these pigments?

85) Zeolites are suitable catalysts for the site-selective catalysis. What could you understand under reagent selective or product selective catalysis at this context? Give an example!

86) Which product do you expect at the reaction of silicon with methyl chloride over a Cu-catalysts?

87) The metastable H_2O_2 is stable in aqueous solution for weeks, but it disintegrates and starts to foam in presence of many contaminates. Explain the reaction for the following catalytic effective substances!

   a. Fe^{3+}

   b. MnO_2

88) The nature uses the catalytic influence of Fe^{2+} for the disintegration of H_2O_2 in cells. Explain the activating influence of haem to H_2O_2 in this context.

89) Explain the concept of photocatalytic water purification in the presence of TiO_2! Make use of a simple sketch and suitable reaction equations!

90) Why are so many metallic catalysts contaminated of sulphur?

91) Which requirement should fulfil a pigment, that it could be used in redox reaction?

92) Which reaction takes place at an auto catalyst? Why is a regulation of the partial pressure of oxygen necessary for an optimal emission control (lambda probe)?

93) Explain the photocatalytic method for water purification!

94) Which method could be used to increase the activity of a catalytic pigment?

95) What is the reason for the increasing influence at the reaction of Mg-Cluster by the Grignard-reagents?

96) In the classical photography emerge a latent picture at first. This presents little unseen nano particular Cluster of a few Ag-atoms, which emerges from the AgBr. These clusters grow by the add- on of reductant at the development process. Explain the reaction mechanism of cluster growth during developing pictures!

97) The wave number of the stretching vibrations of a hydroxyl group is in the range of 3600 – 3660 cm^{-1}. The hydroxyl group is ligated at a Bronstedt center in a metal cation freed zeolite. If the Si/Al ratio increases, it will decrease the frequency of the stretching vibration. Which conclusions can one draw concerning the acidity of the zeolite?

98) Name the application areas of TiO_2? Which modifications will be utilised and why?

99) Explain by a simple sketch the electron flow in a Graetzel cell!

100) In which biological process will be H_2O segregated and the obtained charge (H^+ and electrons) parted efficient?

101) Which type of ceramic do you know?

102) Give two examples for substances, which are used as ceramic.
   a. Binary, oxidic
   b. Ternary, oxidic
   c. Quaternary, oxidic
   d. Binary, nitridic

103) Which properties have ceramics in general?

104) What do you understand under β-aluminium oxide and which ceramics could you deduce out of it? Give two examples for the usage of ceramic materials with β-aluminium oxide structure!

105) At which requirement do you obtain ceramics with good ionic conductivity?

106) What do you understand under scintillator? Give three material classes which could be process to such ceramic.

107) Why are ceramic materials preferred instead of glass for the use as torch in high pressure lamps?

108) Sketch the process of production for (transparent) ceramics.

109) Much ceramic compounds with impurities are like semiconductors. Every vacancy generate a free charge carrier in $Fe_{1-x}O$ (wüstite). Which quantitative composition is necessary to obtain a charge carrier concentration of $5.7*10^{12}$ cm^{-3}? $Fe_{1-x}O$ crystallise in a cubic NaCl-structure (Z = 4) with x = 0.0 - 0.17 and a lattice constant of a = 0.412 nm.

110) Undoped β-aluminium oxide exhibit a maximal conductivity and a minimal threshold energy at a natrium ion surplus of 20 – 30 %. The conductivity decreases with an increasing natrium concentration. Crystals of β-aluminium oxide which are doped with Mg^+-ions have a substantial high conductivity as undoped crystals. Explain these results!

111) What does inorganic glass consist of and how could you describe the structure?

112) Why are glasses transparent or non-light strewing?

113) Which oxides or carbonates must be added at the production of silicate-glass to obtain the following effects?
   a. Decreasing of the melting point
   b. Increasing of the refraction index

c. Increasing of the thermal shock resistance

d. Increasing of the x-ray absorption

e. Decreasing of Hg-consumption in fluorescent lamps

114) Which properties should exhibit a polymer, so that it could transferred easily into glass state?

115) Explain why a surface of fused silica react acid and how can change the acid-base-character because of add-on of network changing components.

116) How could be a glazing with heat protection realised?

117) You should select a sealing glass for a feed-through of an Ultra High Pressure (UHP)-lamp (tungstic wire through a quartz envelope). Which material class would you preferred assay?

118) Which type of glass would you select for a reaction vessel, if you perform photochemistry with a Hg- high pressure lamp as radiation source?

119) How could you displace the absorption edge of soda-lime glass into blue by change of composition?

120) How could you obtain glasses with a high electric conductivity?

121) How emerge a blurring of glasses and could it be prevented?

122) Radiant glasses have been produced with add-ons of ZnS:Cu an radioactive ions in the early 20^{th} century. Which ions will be offered and how can a permanent luminescence of glasses be achieved?

123) Which ions do you choose to dope the appropriate glass to obtain the following effects?

a. Image screen with a better contrast

b. Halogen lamps without UV emission

c. Glasses with photochromism

124) How could you verify, whether a substance is amorphous or vitreous/glassy?

125) Explain the effect of Na^+ or K^+ to the softening point of glass with simple reaction equations! Which effect do you expect by the addition of B_2O_3?