Clausur Questions
for Theo.Chem. I

TC, 1a)
Given 2 functions $p_x = f\cdot\cos\varphi$ und $p_y = f\cdot\sin\varphi$. The range of angles is $\varphi \in [0,2\pi]$. Normalize p_x to 1. What is $\langle p_x | p_y \rangle$? (Try to apply only simple arguments.) What does this result mean?
TC, 1b)
For each observable, measurable quantity x, there is a corresponding operator **X**. E.g. if you choose, for position x, the operator **X** = x· ; then, for momentum p, the operator is **P** = ... All these operators must have some peculiar mathematical property/ies. Which one(s)?
TC, 1c)
Give the definition of a Hermitean operator A . Which property do its eigenvalues have?

TC, 2a)
Compare (**I**) $[R_2\underline{N}–CH=CH–CH=CH–CH=NR_2]^+ClO_4^-$, (**II**) $[R_2N=CH–CH=\underline{N}–CH=CH–\underline{N}R_2]^+ClO_4^-$. How many π-pairs does **I** : and **II** : have ? Which one of the two compounds absorbs light of smaller frequency?
TC, 2b)
How does the wave number $\nu = 1/\lambda$ of the first absorption band, of a conjugated π chain with equal bond lengths D and number N of atoms in the chain contributing 1 π electron each, in the VIS-UV region vary with the length L = (N+1)D of the chain? Sketch a diagram. Can you derive the relation using the model of an electron in a box?
TC, 2c)
If the wave number number is $\nu = 20\cdot10^3$ per cm, then the wave length is λ =

The energy of the respective photons is eV.

This corresponds to an energy of kJ/mol.

TC, 3a)
An experimentalist measures the angular momentum component L_x of atomic particles along the x-axis. He obtains a statistical collection of only three different values: ≈ 1 ħ , or ≈ - 1 ħ , or ≈ 0 ħ . Give the value of the angular momentum vector, which characterizes these particles: l = ... ,
Give the value of the total angular momentum, |L| = ...
TC, 3b)
Which type of 2-electrons positional state function $\boldsymbol{\psi(r_1,r_2)}$ may be combined with the 2-electrons spin direction state function $\boldsymbol{\chi(s_1,s_2) = \alpha(s_1)\cdot\beta(s_2) + \beta(s_1)\cdot\alpha(s_2)}$? Give an explicit example for $\boldsymbol{\psi(r_1,r_2)}$.
TC, 3c)
Does the spin function $\boldsymbol{\chi(s_1,s_2)}$ from (3b) describe two parallel or two antiparallel spin vectors?
Draw a graphical sketch.
TC, 3d)
Explain the mechanism of covalent bonding.

Colloq, a)
Gold Nanoparticles: Typically they consist of how many atoms? Give a range N: ....
How can one prevent the Au_N cluster particles to form bigger colloidal particles?
Colloq, b)
Sketch the setup to measure the electric conductivity of single molecules .
Which molecules, for instance, are interesting in this context?
Colloq, c)
How does the fluorescence spectrum of a semiconductor nanoparticle look like?
Of a single quantum dot? Of a surface covered with many of them?

Surface, a)

You fill a plastic box with a hole at the bottom with water until the water starts to run out of the hole. This hole has a radius of 0.1 mm. As you know the height of the water level is 14.7 cm. You add a substance which dissolves in the water. The final concentration is 100 mMol/l. You observe that the water starts to run out of the box again until it reaches a height of 12 cm. The temperature is 25°C. - What is the surface tension after adding the substance?

Surface, b)

Please estimate the surface excess in molecules per nm^2.

Surface, c)

Instead of adding the substance, you heat the water to 40°C. Does water run out (starting from a height of 14.7 cm)? If yes, to which level does it run out?