# CHE502 Chemical and Statistical Thermodynamics
# Fall semester 2021

Sept. 27 - Oct. 8 2021, 14.00h - 17.00h Thailand time

via ZOOM

URL: http://theo.ism.u-bordeaux.fr/PBopp/vistec.2021.2022

**Aj. Montree, Aj. Michael, and Aj. Philippe**

michael.probst@uibk.ac.at philippebopp@yahoo.com
montree.s@vistec.ac.th


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Signal De Botrange
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Prague
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Paris
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Vienna
Munich
Feldberg
AUSTRIA
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Zugspitze
Grossglockner
SWITZERLAND
Vaduz
Bern
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Geneva
Ljubljana
Monte Rosa
Puy De Sancy
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Pico De Aneto
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SPAIN
Monte Cinto
Mediterranean Sea
Rome

– This is the second time that we teach this class remotely via ZOOM
– Even though this is certainly not as good as teaching face to face,
we think it worked out quite all right for "batch 6" last year.
So we'll try to make the best out ot it again.

We have this year (according to the list we got)
4 chemists, 4 chemical engineers, and 2 physicists
coming from 4 (or 5, depending how we count Kamphaeng Saen) Universities

This is quite heterogenous, so we'll need to spend some time creating a (more or less) common background for everybody.
This means that, depending on the knowledge you already have, you will have to study different things in the beginning (this introduction).

–The class will thus be essentially structured as follows:

- After some introduction by Michael and/or Philippe
  students will be given a reading assignment for the next class
  students will prepare a list of questions to be discussed

- We have prepared lecture notes for each topic,
  which also contain references to textbooks
  (see also the links on the web page
  http://theo.ism.u-bordeaux.fr/PBopp/vistec.2021.2022/)

- The following session will start with a general discussion
  of the reading assignment

The powers that be have decided that there must be an exam,
so we'll have a written exam at the end of the class (90 minutes or so).

The exam will be open-book (actually open-everything (incl.GOOGLE,
we always can find questions which are not on GOOGLE 555))

We will send you the questions (LibreOffice (WORD) doc or docx file
by e-mail before the exam starts
You fill in the answers
  and send back the file at the end of the exam

The **aims and purposes** of this series of classes (CHI502 CHI501) are manyfold

– Learn to understand spoken English

*unfortunately this year this purpose will not be served too well*

– Learn to speak (ask questions) and write in English

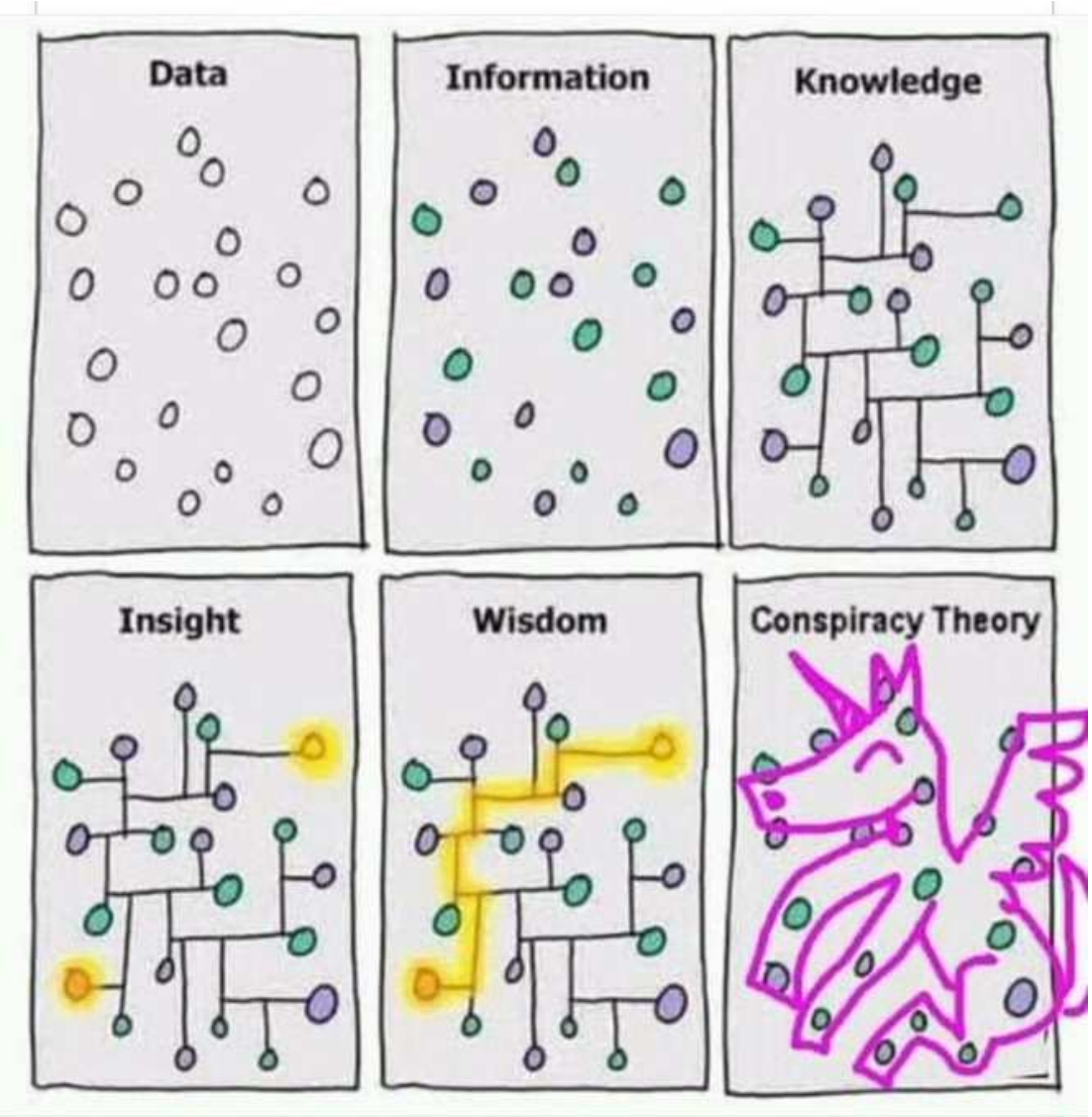
– Learn about Science and Research in general

Get to know some fundamental concepts that one needs to master in all sciences, such as:

"Approximation", "coarse graining", "effective", "level of theory" "phenomenological", "model", and many others

– Allways stay curious, open-minded, and critical!

"Wenn wir wüssten, was wir tun, würde man es nicht Forschung nennen"
(If we knew what we are doing, it would not be called research) (Einstein)




Science is not just collecting data, but **understanding** them

This means you need theory (laws)

The question: "what does it mean to 'understand'" is a very difficult one
(Epistemology, the science of 'knowledge')
It cannot be fully answered here, just a few keywords:
–An "explanation" should reproduce the known facts
–An "explanation" should be as simple as possible (known as Occam's razor)
–An "explanation" should be free of contradictions
–An "explanation" should allow to make predictions of future results
(which means there MUST be a way to prove it wrong (falsifiability) )

*A little joke*
*An engineer builds a bridge. Probably the bridge will not collapse*
*The engineer has no idea why the bridge does not collapse*
*A physicist builds a bridge. May be the bridge will collapse*
*The physicist knows exactly why the bridge collapsed*

## Falsifiability

**This is a very important principle in science**

- Only a statement that can be demonstrated to be wrong
  is a scientific statement

- This means for instance:
  When you write a scientific paper, or a report, or anything similar,
  you MUST of course say the truth,
  but you MUST also provide all details so that anybody can check
  your work (by repeating it) and see whether it is correct or not
  ($\rightarrow$ reproducibility)
- In other words:
  **A scientific paper is neither an advertisement nor a propaganda brochure**

In this class, we will start to build systematically such an understanding of (some) chemistry
starting at the level of individual molecules and moving on to
assemblies of molecules, including very large assemblies
(called condensed phases, ie. liquids, solids)

We will also see how to make use of experiments (such as spectroscopies) toward this aim

For this purpose, we will look at (hopefully review for most of you)

– Characteristics of molecules, dimensions, energies
  (Nuclei, protons, neutrons, electrons, electronic spins, nuclear spins, ..)
  which ones are important in chemistry, what are the energies involved,
  how do these energies appear in the electromagnetic spectrum
  (as a carrier of energy)? How is this energy transferred?

We also need to recall* the basics of Quantum Mechanics (QM)

Why QM? Where does it apply?

Can some simplifications/assumptions be made when it is used in chemistry (ie. in the range of 'chemical' energies)?

What do experiments say? How can we 'understand' them? (phenomenological thermodynamics, IR and Raman spectroscopies, various NMR techniques, X-ray (and neutron) scattering etc)

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* *Those of you who followed an undergraduate curriculum (eg. in some kind of engineering) that does not include a class entitled something like: 'quantum mechanics', 'quantum chemistry', 'quantum physics', 'chemical bonding', some 'physical chemistry' (depending on university) will have to do a lot of reading for this topic. Contact Michael or Philippe if this is the case.*

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At this point we will have a brief look at some numeric/computational aspects

Nowadays any type of 'interesting' calculation can be done only by using computer programs (or codes)
These codes are either freely available, or must be purchased, or everyone has to write them themselves

– Do you know any programming language?
  (Python, mathlab, FORTRAN, c, C++, PASCAL, .....)
– To show and discuss your results, you will also need to master
  some graphics software
  *one picture is worth 1,000 words, they say*

We will not go very deeply into this and just look at a few examples of typical techniques to highlight their potential,
but also the inherent difficulties and limitations

May be in CHE501 we will be able to do a little practical work

Then we need to tackle a little bit of Statistical Mechanics
(*Note: Statistical Mechanics is much easier to understand if one knows QM*)

This will lead us toward CHI501
– Statistical Mechanics, concept, phase space
– Statistical Mechanics via molecular simulations
– Modeling
– A few necessary approximations & tricks
– Extracting information from simulations
– Statics (thermodynamics)
– Dynamics (kinetics)

If time permits:Other Simulation Methods
Examples, Computer Lab

There are many books available to you in the VISTEC library, unfortunately usually only one copy.

General physical chemistry

| | | |
|---|---|---|
| QD 453.3 A873P 2010 | Physical chemistry | Atkins, P. W. |
| QD 453.3 A873P 2014 | Physical chemistry : thermodynamics, structure, and change | Atkins, P. W. |
| QD 453.3 E57P 2014 | Physical chemistry | Engel, Thomas |
| QD 453 M821P 1966 | Physical chemistry | Moore, Walter J |
| QD 453.2 B278P 1979 | Physical chemistry | Barrow, Gordon M |

The books by P.W.Atkins are highly recommended.
The books by Moore and Barrow are a bit older
There are also many other physical-chemistry textbooks, e.g. the one by Berry/Rice/Ross (may be a bit of overkill for you),
the one by Ira Levine (excellent) ...

## Quantum mechanics/physics/chemistry

| | | |
|---|---|---|
| QD 462 M478Q 2008 | Quantum chemistry | McQuarrie, Donald A. |
| QC 174.12 G824Q 1998 | Quantum mechanics. | Greiner, Walter |
| QD 461 AT873A 2003 | Atkins' molecules | Atkins, P. W. |
| QD 462 A873M 2011 | Molecular quantum mechanics | Atkins, P. W |

There is also an excellent Quantum Chemistry textbook by Ira Levine

## Statistical mechanics/simulations

| | | |
|---|---|---|
| QC 174.8 M478S 2000 | Statistical mechanics | McQuarrie, Donald |
| QC 173.457 .C64 R37A 2004 | The art of molecular dynamics simulation | Rapaport, D. C |
| QD 455.3.E4 J46 2017 | Introduction to computational chemistry | Jensen, Frank, |
| QD 480 L43 2001 | Molecular modelling :principles and applications | Andrew R. Leach |

An older textbook on simulations, by Allen and Tildesley is now in the public domain and available on the web

Specific experimental methods

| | | |
|---|---|---|
| QC 454.V5 W747M 1955 | Molecular vibrations : the theory of infrared and Raman vibrational spectra | Wilson,Decius,Cross |
| QD 945 W913i 1997 | An introduction to X-ray crystallography | Woolfson, M- M. |

The book by Wilson et al. is the 'bible' of al vibrational specroscopists

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$\Longrightarrow$ You can find excellent* lecture notes and videos,
and I think now also textbooks (all in Thai),
on Aj. Teepanis Chachiyo's (Naresunan University) web site
(https://sites.google.com/site/siamphysics/) 'Siam Physics'
check in particular
– Classical Mechanics – Quantum Mechanics,
– Numerical Methods – Statistical Mechanics

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* *of course I cannot read anything, but the figures, and the order in which they appear, seems very close to what we will do here*

More books

C. Kittel, Introduction to Solid State Physics, Wiley
*The title says it all*

R.K. Pathria (and P.D. Beale in later editions)
Statistical Mechanics, Elsevier
http://home.basu.ac.ir/~psu/Books/[Pathria_R.K.,_Beale_P.D.]_Statistical_mechanics.pdf
*for the introduction to the concept of 'partition function'*
*starting from quantum mechanics*

M.P. Allen, D.J. Tildesley,
Computer Simulation of Liquids, Oxford Science
*detailed explanations of the fundamentals, with FORTRAN codes*
http://www.ccl.net/cca/software/SOURCES/FORTRAN/allen-tildesley-book/f.00.shtml

I.R. Levine, Quantum chemistry, Prentise Hall
*one of my favorite QC books*
http://www.slideshare.net/diegogarciadossantos/0835quantum-chemistry-5th-edition-by-ira-n-levine

More free books at:
http://www.freebookcentre.net/Chemistry/Quantum-Chemistry-Books.html