CHE502 Chemical and Statistical Thermodynamics
Fall semester 2020/2021
Tuesday afternoon 14.00h - 17.00h

URL: http://theo.ism.u-bordeaux.fr/PBopp/vistec.2020.2021

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SPAIN
Monte Cinto
Mediterranean Sea
Rome

– This is the first time that this class (and in spring CHI501) will be taught remotely via ZOOM

– This is certainly not as good as teaching face to face, but we will try to make the best out of it.

–The class will thus be essentially structured as follows:

(1) Michael and/or Philippe will give a short introduction to a topic

(2) - Students will be given a reading assignment until the following week

- Students will prepare a list of questions to be discussed

- We will prepare lecture notes for each topic

(see http://theo.ism.u-bordeaux.fr/PBopp/vistec.2020.2021/)

(see also the lecture notes from previous years here)

(3) The following session will start with a general discussion

(4) Back to (1)

But first we need to get to know you

Please prepare a list with
–your name
–your little name (if you like, it's easier for us to remember!)
–from which university you graduated
–your major there (physics? chemistry? math? bio....??? ....?)
–with which VISTEC adjarn you think you will work

Since we are probably not very numerous (and also flexible) this info will allow us to tailor a little bit what we teach.

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.

Exam

We are not sure yet how we'll do it.

We'll probably send a problem/question sheet to Aj.Montree,

who will run the exam (not too long, 2 hours may be) in the usual vistec fashion

We strongly prefer open book / open Internet exams,

i.e you can consult what you want (an English-Thai dictionary, your favorite textbook, the lecture notes, ...) during the exam.

BEWARE: This does not make the exam easier, but harder!

(*since we ask, of course, questions that cannot be GOOGLEd,*

where you need to think, not just to memorize)

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

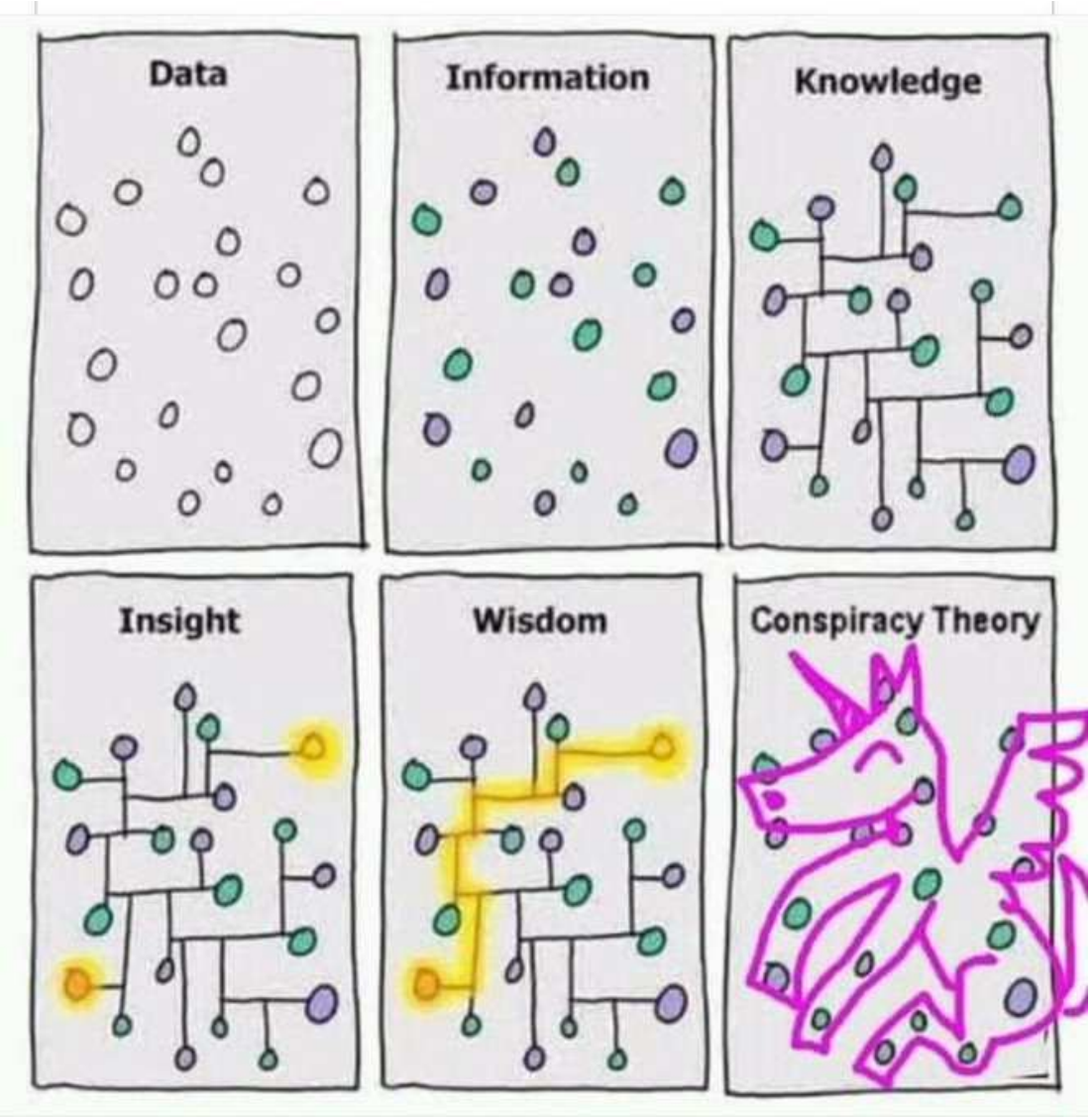
Get to know some concepts that one needs to master
in all fundamental sciences, such as:
"Approximation", "coarse graining", "phenomenological", "effective",
"model", and many others

– Stay critical, curious, and open-minded

"Wenn wir wüssten, was wir tun, würde man es nicht Forschung nennen"

(Einstein)

(If we knew what we are doing, it would not be called research)



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 thus 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 not including a class entitled something like:*
'quantum mechanics', 'quantum chemistry', 'quantum physics', 'chemical bonding', some 'physical chemistry' classes (depending on university) will have to do a lot of reading for this topic

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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