Computers in Chemistry – Lecture I

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Nagoya University

What you need for this class

- Nagoya University ID, e.g.:
- Your password
- In case of problems or questions, please contact: sirle@chem.nagoya-u.ac.jp (also on your hand-out)
- Prof. Irle's office hours: Mondays, 13:00-14:30, location: SA building, 4th floor, 424.
- Student TA in this class: Hong En Lim, E-Mail: lim.hong.en@b.mbox.nagoya-u.ac.jp

This class (handouts)

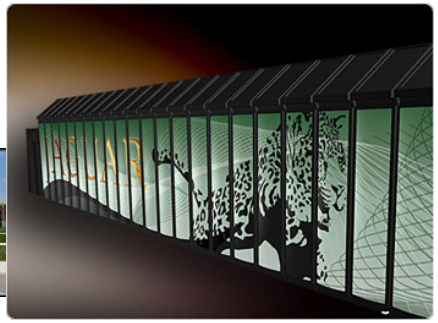
- Please check: http://qc.chem.nagoya-u.ac.jp
- Click on "Teaching"
- Username: qcguest, password: qcigf! (memorization help: quantum chemistry is great fun!)

(today the Department website does not work due to hacker attack on Nagoya University's website)

The general contents of this class

- **Question**: *Why FORTRAN 90?*
- **Answer**: According to Robert Harrison, Director, Joint Institute for Computational Sciences (USA):
  - Not "old"
  - 70% of applications in FORTRAN

www.jics.utk.edu



What is chemistry? I

First in use: 1646

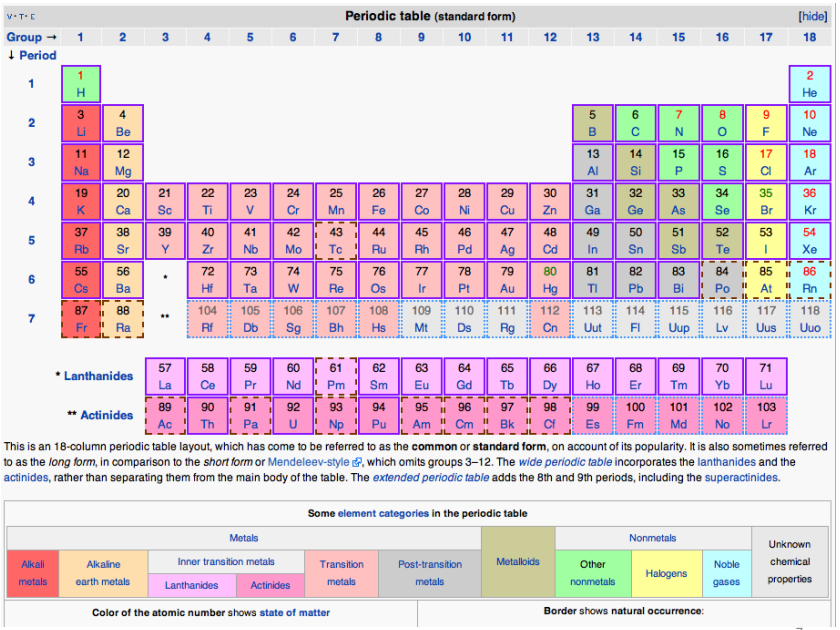
- **Answer I** (commonly quoted): Chemistry is the study of **matter** and **energy** and the interactions between them.
- **Answer II** (Webster's dictionary):

  a) the science that deals with composition, structure, and properties and with the **transformations** that they undergo

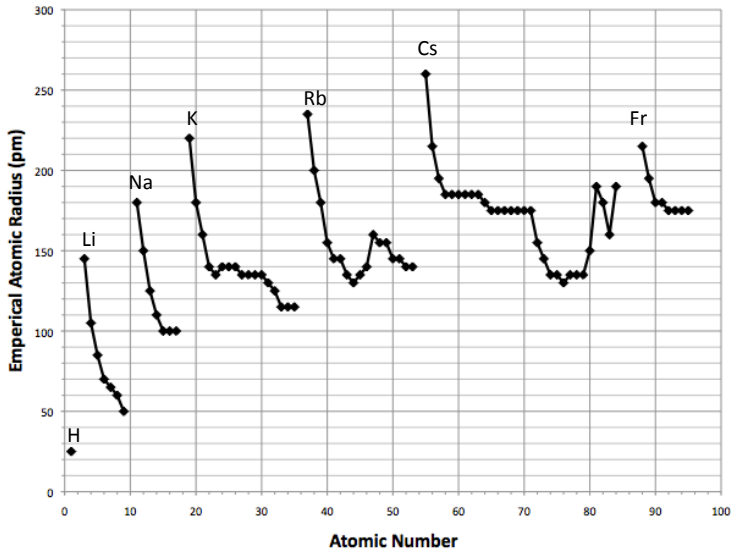
  b) a strong mutual attraction, attachment, or sympathy ("this couple has a great chemistry")

- Alchemists: Ignis mutat rei (Latin: Fire changes matter)
- Goal: Change lead into gold (Pb → Au)

The Explosion in the Alchemist's LaboratoryJustus Gustav van Bentum (Leiden 1670–1727) Holland, 17th or 18th century Oil on canvas



http://en.wikipedia.org/wiki/Periodic_table



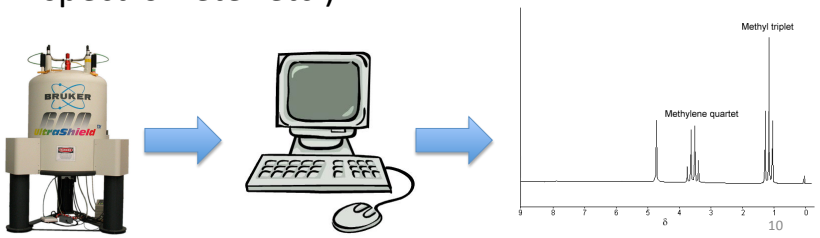
Atomic DATA
http://en.wikipedia.org/wiki/Periodic_table

Chemistry is the "Study of Change"

- Chemistry of the **Universe** (interstellar clouds)
- Chemistry of the **Earth** (geological chemistry)
- **Darwinian Evolution** (biochemistry)
- Chemistry of **Nature** (Organic/inorganic chemistry, physical chemistry, analytical chemistry [**collect knowledge**])
- Chemistry of **Man** (Medical chemistry, chemical technology [**apply knowledge**])

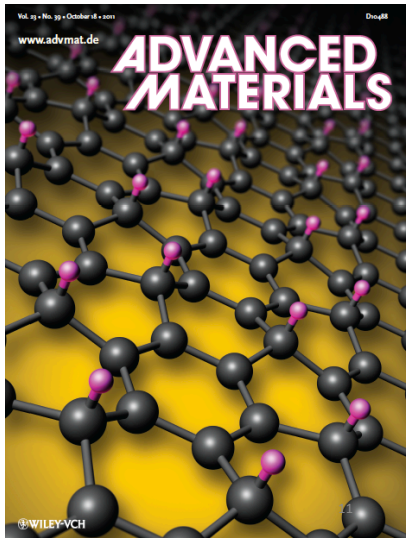
Computers in Chemistry?

- Finding DATA in literature or databases
- Produce DATA (theoretical/computational chemistry)
- Analyze DATA (computer attached to spectrometer etc.)



Chemical Knowledge

- Papers written in books and scientific journals
- Peer-reviewed
- Open-access?
- Many many journals
- Many, many studies
- **Science nowadays is run like a business!**



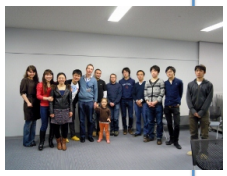
Chemical Knowledge

- Impact factor of a journal

Mark	Rank	Abbreviated Journal Title (linked to journal information)	ISSN	JCR Data						Eigenfactor™ Metrics	
				Total Cites	Impact Factor	5-Year Impact Factor	Immediacy Index	Articles	Cited Half-life	Eigenfactor™ Score	Article Influence™ Score
☐	1	ACCOUNTS CHEM RES	0001-4842	33869	21.852	20.330	3.235	149	7.4	0.09692	7.076
☐	2	ACS NANO	1936-0851	9914	9.865	9.962	1.478	986	1.8	0.05575	3.393
☐	3	ACTA CHIM SINICA	0567-7351	2287	0.611	0.586	0.043	415	4.9	0.00319	0.072
☐	4	ACTA CHIM SLOV	1318-0207	959	1.011	1.233	0.076	132	4.1	0.00340	0.311
☐	5	ACTA PHARMACOL SIN	1671-4083	4364	1.909	2.033	0.338	207	5.8	0.01005	0.484
☐	6	ACTUAL CHIMIQUE	0151-9093	116	0.145	0.125	0.012	82	5.3	0.00036	0.039
☐	7	ADV FUNCT MATER	1616-301X	22516	8.508	9.442	1.202	481	3.8	0.11097	3.075
☐	8	ADV MATER	0935-9648	68115	10.880	11.306	2.097	777	5.2	0.24245	3.765
☐	9	AFINIDAD	0001-	183	0.233	0.244	0.000	21	7.0	0.00028	0.044

Chemical Science as a Business

Schematic flow-chart for the research of a chemistry professor



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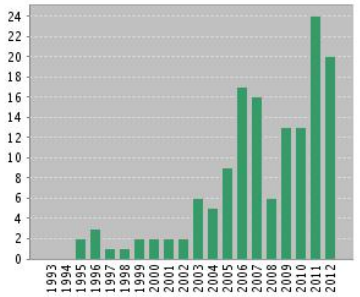
- Perform research
- Write papers
- ***Give talks, get cited by others***
- Write proposal to government agency (JSPS, NSF, DFG, …)
- Get more money
- Hire more people
- Perform more research
- Go to 10

Deutsche Forschungsgemeinschaft

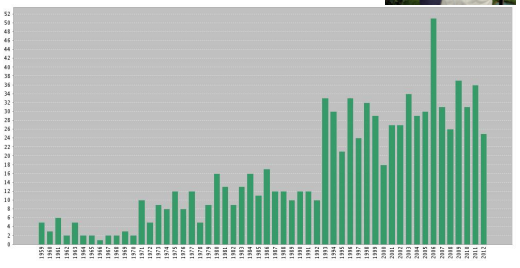
Chemical Science as a Business

Number of papers of a researcher as function of time

Irle, S* (45)



Morokuma, K* (78)



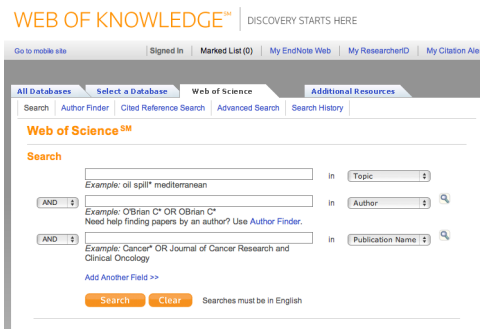
Japan Science and Technology Agency

Moved to USA

Chemistry Knowledge

- How to find chemistry papers?
- - ISI Web of Knowledge

http://www.webofknowledge.com/WOS



Chemistry Knowledge

- Databases
  - Example: QCLDB II

http://qcldb2.ims.ac.jp

Chemistry Knowledge

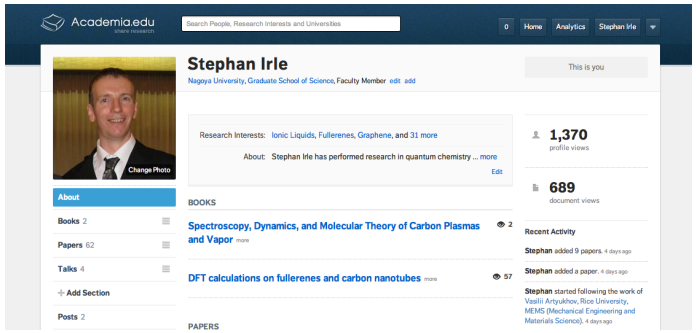
- How to access journals
  - Nagoya University electronic journals
    http://sfx.nul.nagoya-u.ac.jp/nagoya/az/

Chemistry Knowledge

- Social Networks
  - For instance, Facebook
    http://www.facebook.com

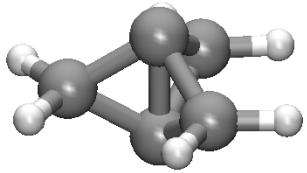
Chemistry Knowledge

- Social Networks
  - 2nd Example: academia.edu (pushes publications up in Google searches), others: ResearchGate.com



Interactive Task:

- Find a research paper on the [1.1.1]propellane (C_5H_6) molecule.



- Write on the back of the Assignment I sheet:
- a) the name of the paper, and
- b) how you found this paper.