Using data-driven exercises in General Chemistry to assess self-regulation and tolerance of ambiguity

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http://goo.gl/55EFop

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President's Council of Advisors on Science and Technology (PCAST) 2010:
instructors during the first two years of college must focus on deeper and transferable knowledge

Quoting the NRC "Framework for Science Education":
"Analyzing and interpreting data", "engaging in argumentation from evidence", and "evaluating information" can all be seen as distinct components of critical thinking. **J. Chem. Educ. 2016, 93, 799−800**

P. Atkins. Pure Appl. Chem., Vol. 71, No. 6, pp. 927-929, 1999.
"…we should teach them to judge between conflicting influences. That is the essence of our subject, for it is rare that a single property governs the outcome of a reaction. We need to train our students to judge the likely outcome of conflict"

"…I assume there are exceptions to this rule because there is an exception to pretty much every rule in chemistry." **Gen Chem student.**

Outline

Curriculum

Structure-property relationships in General Chemistry

Objectives

Low order

Higher order cognitive skills (HOCS)

Control Variable Strategy (CVS)

Self-regulation

Tolerance of ambiguity

Implementation

Data-driven exercises on the web. ChemEd X Data

"Conflicting factors" questions

Analysis

Cheminformatics tools

Sankey diagrams
Cluster analysis

Structure-property relationships in 1st semester of General Chemistry

Properties of Substance — Substances — Electronic or molecular structure

$$Y \leftrightarrow A\,X$$

(it's never one single factor … and sometimes they come into conflict)

Electronic ground state of elements	↔	Aufbau principle + Hund's rule
Atomic size and ionization energy	↔	Nuclear charge + shielding + orbital size
Ionic lattice energy of crystal solids	↔	Cation's and anion's size and charge
Boiling point of molecular solids	↔	Intermolecular forces + shape + mass
Heat capacity of molecular solids	↔	Intermolecular forces + bonds + mass

Assignments for HOCS in structure-property relationships: Y = AX

- [Y,A] → X **Self-regulation**
  Given a set of substances (A) and their properties (Y) <u>discover</u> what the deciding structural factors are (X).
- [Y,A] $\overset{?}{\Leftrightarrow}$ [X] **Ambiguity+Conf. factors**
  Given a set of factors that may intervene in the property of substances [A], <u>identify</u> the deciding factor that prevails.
- [A,X] $\not\rightarrow$ [Y] **Ambiguity+Conf. factors**
  Given a set of substances (A) and their structural factors (X), identify the cases when you <u>can't predict</u> (Y).
- [X,Y] → A **Self-regulation**
  Given that a property (Y) is affected by factors (X), come up with a list of substances (A) that <u>show evidence</u> of the relationship

Higher order skills in Gen. Chem.

Properties of Substance Substances Electronic or molecular structure

$$Y \leftrightarrow A\ X$$

Tolerance of ambiguity: conflicting factors

Atomic size and ionization
- Nuclear charge
- Electronic shielding
- Orbital size

Example Radius:
r(O) < r(Cl)
r(Li) > r(Mg)

Boiling points
- Mass
- Shape
- Intermolecular forces

Example BP:
$CH_2F_2 > CF_4$
$CH_2Cl_2 < CCl_4$

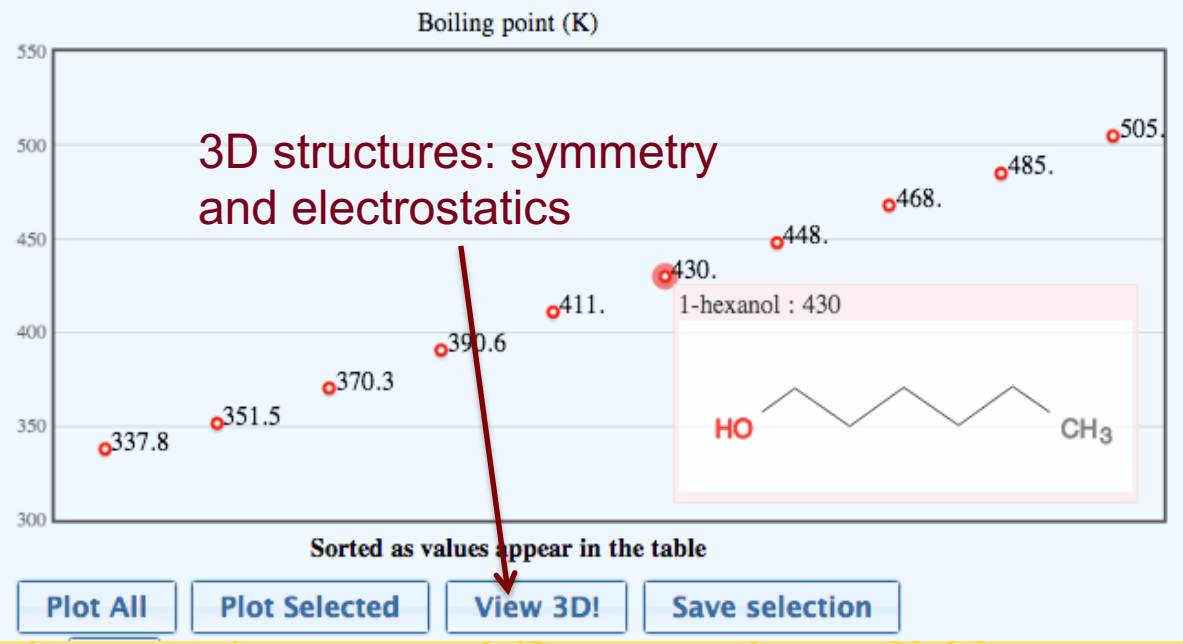
Self-regulation: control of variables strategy and interpretation

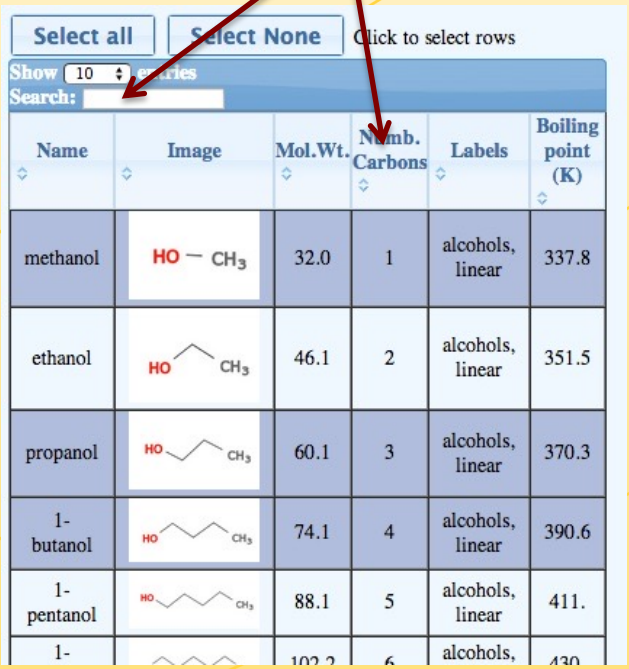
Using unstructured data, easy to navigate, select and represent to build “controlled experiments” and identify trends and exceptions.

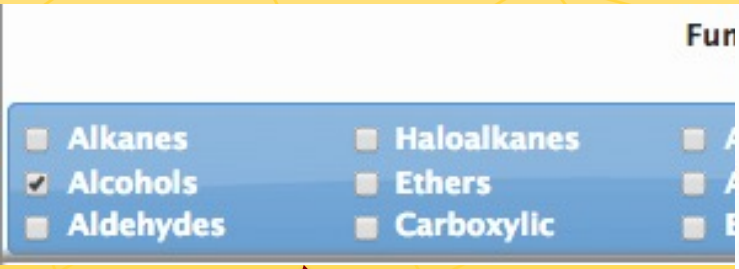
ChemEd X Data http://chemdata.r.umn.edu
J. Chem. Educ., 91(9), 1501-1504, 2014

http://chemdata.r.umn.edu

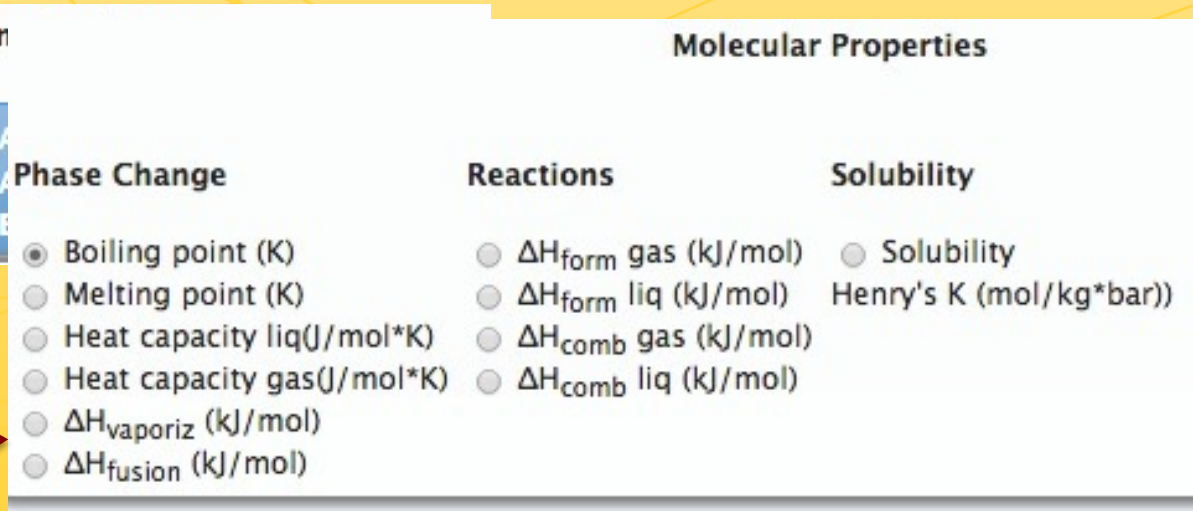
Order and filter







Select func. groups and properties



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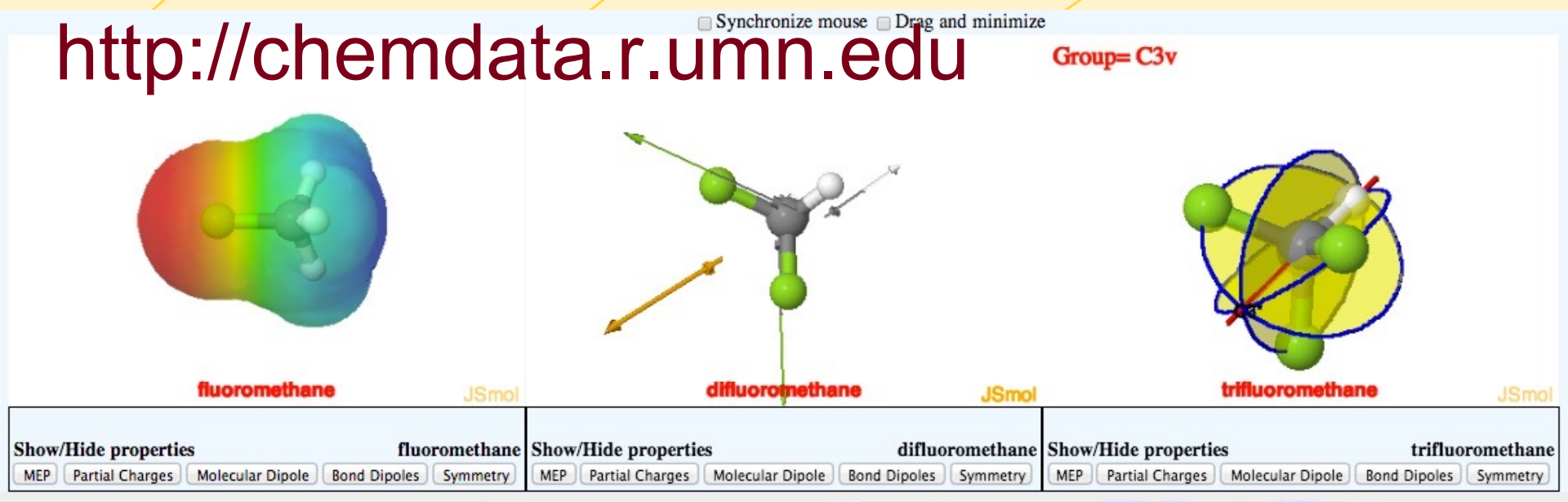

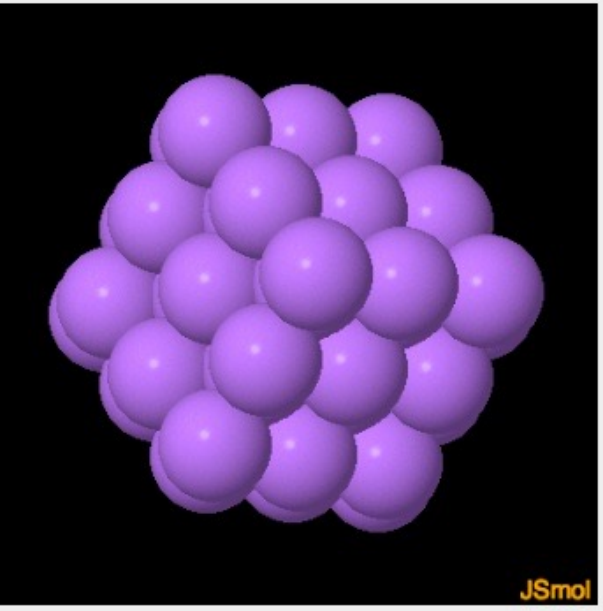

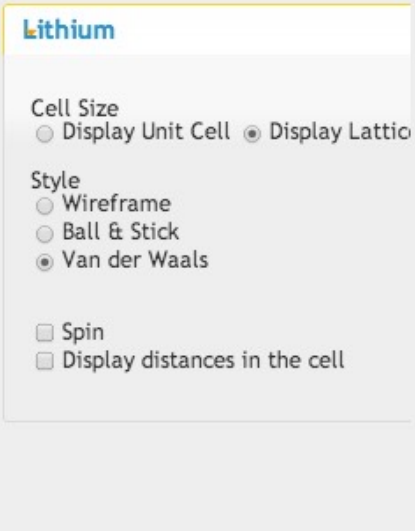

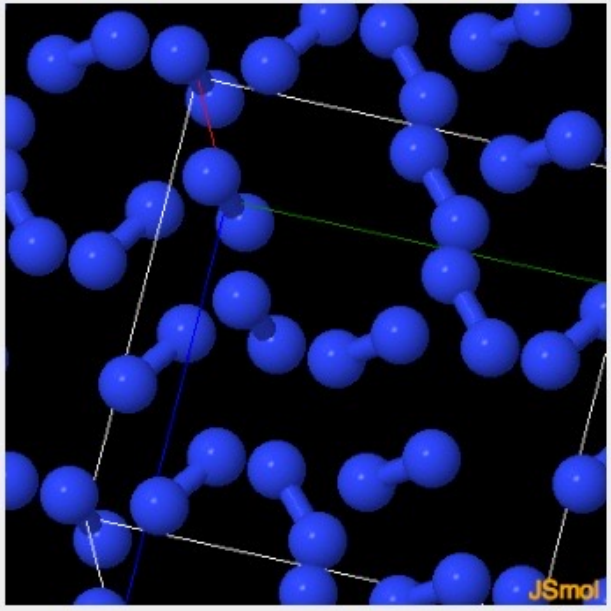

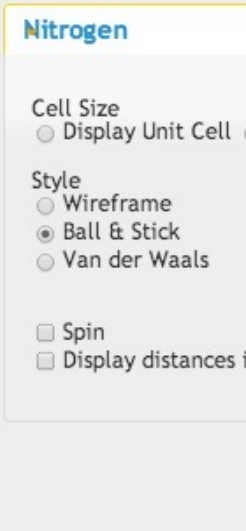

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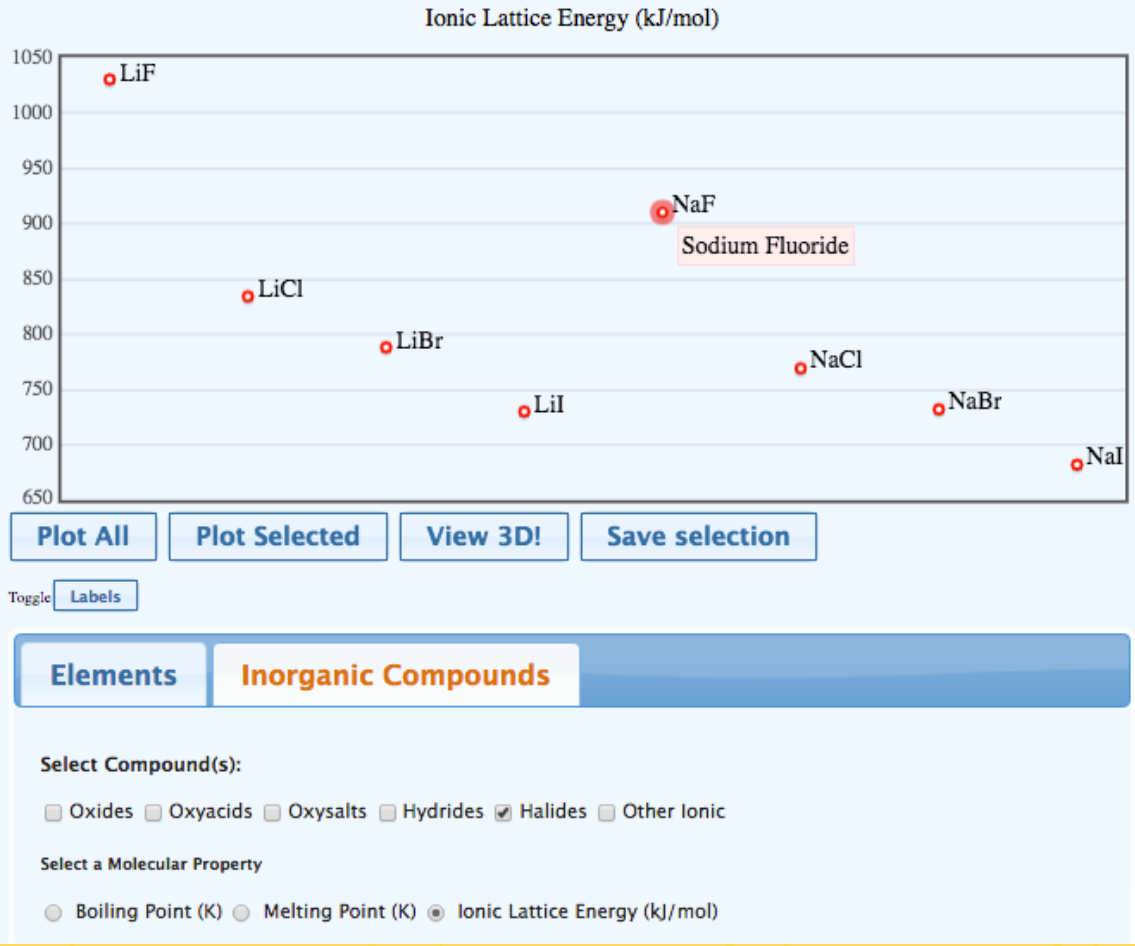
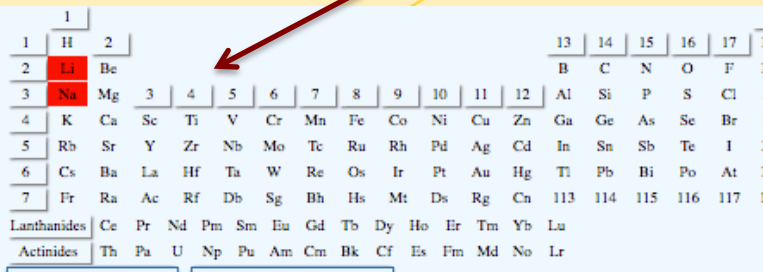
Periodic table for easy selection





Select All | Select None | Click to Select Rows

Show 100 entries

Search:

Name	Formula	Compound Label	Ionic Lattice Energy (kJ/mol)
Lithium Fluoride	LiF	Halide	1030
Lithium Chloride	LiCl	Halide	834
Lithium Bromide	LiBr	Halide	788
Lithium Iodide	LiI	Halide	730
Sodium Fluoride	NaF	Halide	910
Sodium Chloride	NaCl	Halide	769
Sodium Bromide	NaBr	Halide	732

ChemEd X Data http://chemdata.r.umn.edu

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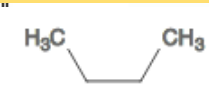
Can students do CVS and analysis?

Assignment: Select a set of compounds that help us understand the effect of mass and molecular shape on the boiling point.

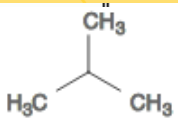
Builds a valid "controlled experiment"
Interpretation of data is consistent with selection?

Effect of mass	
69.8 % yes	30.2% no
88% yes	12 % no

Shape effect: linear/branched		
40 % yes	60% no	
40% yes	44% ambiguous	16% contradict

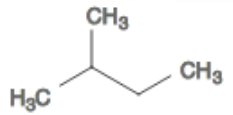


Mass: 58.1222; BP=273.

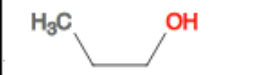


Mass: 58.1222; BP=262.

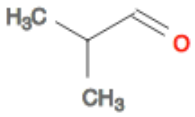
Mass: 72.14878; BP=309.2



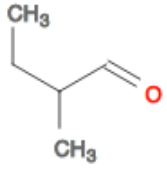
Mass: 72.14878; BP=301.1



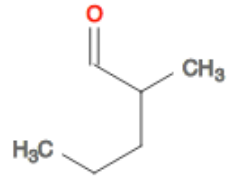
Mass: 60.09502; BP=370.3



Mass: 72.10572; BP=336.



Mass: 86.1323; BP=365.



Mass: 100.15888; BP=391

CVS and identify limit of predictability

Name	Mass	BP (°C)
Methanol	32	338
Butane	58	273
Octane	114	399

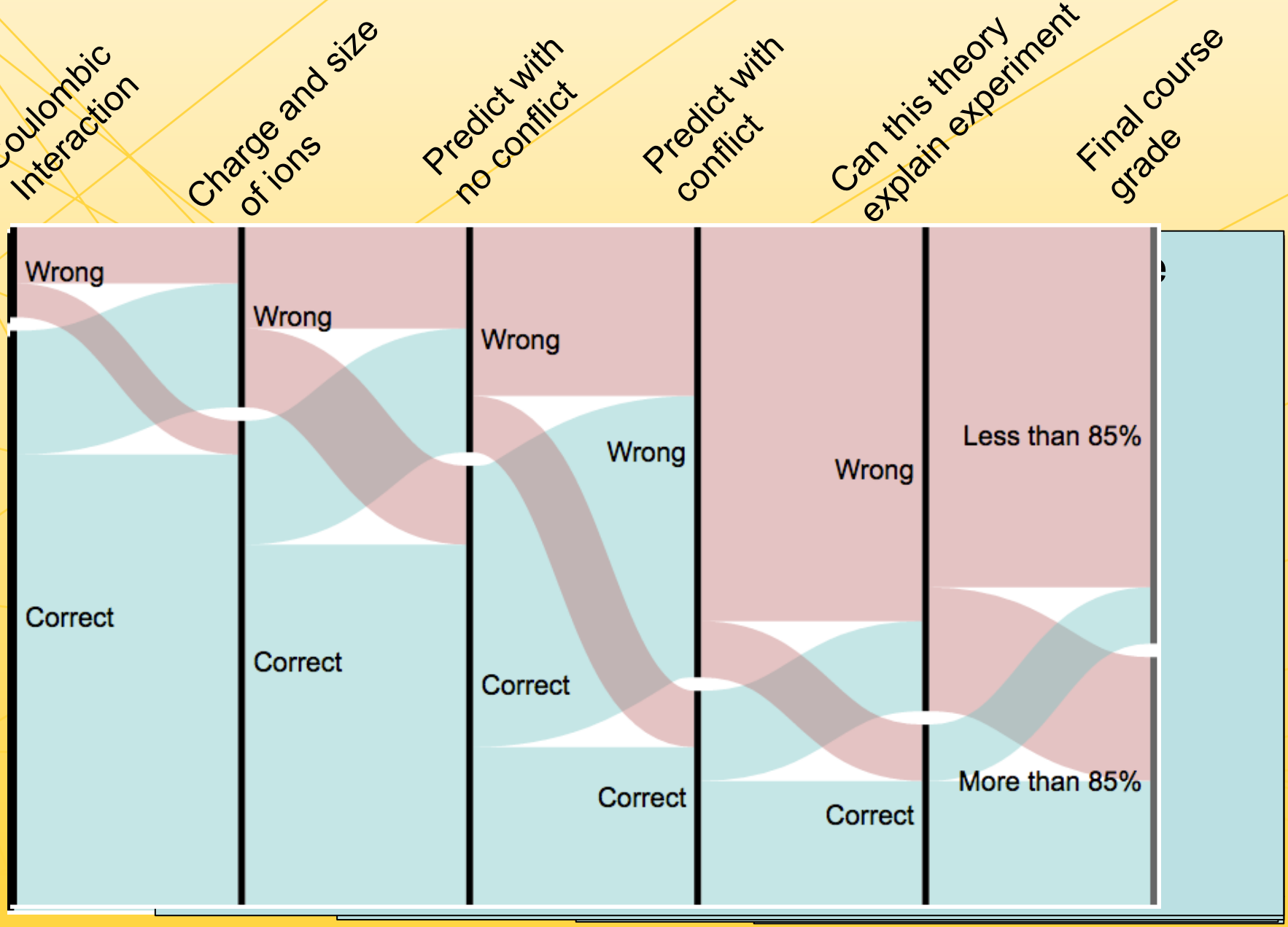
http://chemdata.umr.umn.edu/chemedXdata/index.html#stamp=1470068542409

Assignment: What has a stronger influence, a heavy molecule with a weak intermolecular force or a light molecule with a strong intermolecular force? Are there exceptions?

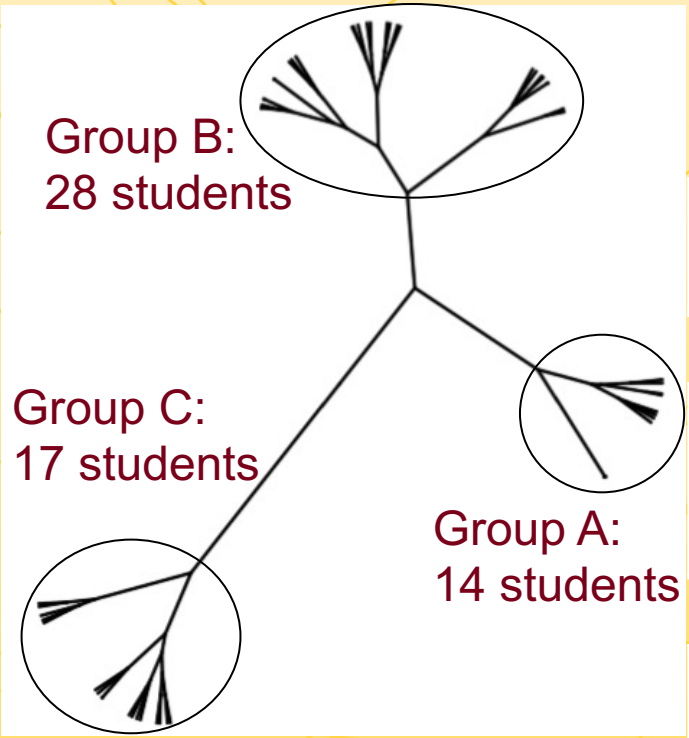
Mass or IMF?	Mass vs IMF	
	60.3 % mass	39.7% no
Provide valid evidence of their statement?	50.8% yes	49.2% no

- 39.7% was inconclusive.
- 9% say no exceptions.
- The “new site” effect may add noise to the results

Can students recognize “conflicting factors”?



Clustering survey results



	Group B n = 28	Group C n = 17	Group A n = 14
Course Grade	81.0±9.2	79.0±6.2	88.0±5.5
Ionic energy survey	62.7±14.2	31.7±9.3	88.1±12.9
Conflicting factors questions	14.3±26.2	8.8±19.1	85.7±22.6

Hierarchical cluster analysis (Ward's minimum variance method) using the results for the "Ionic lattice energy" survey

Conclusions

- We have used data-driven exercises to address “controlled variable skills” and “self-regulation.
  - It is challenging to offer students “unstructured data” without a steep learning curve to navigate it.
  - ChemEdXData is now available on GSpreadSheets.
- Identifying conflicting factors and the limit of predictability depends on previous knowledge and it is a HOCS.
  - With a Sankey diagram we can see the progression
  - With clustering analysis we can group the students and see how HOCS relates to their grade

ChemEdXData on GSpreadsheets