Using data-first activities on the web to practice structure-property relationships

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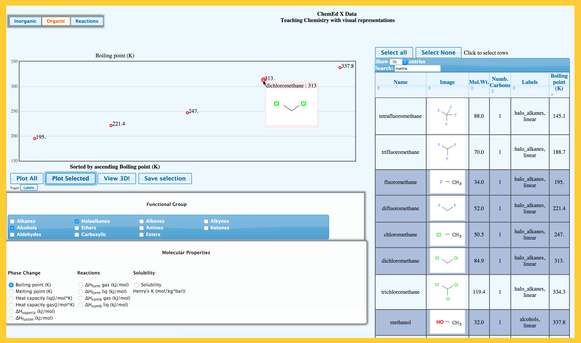
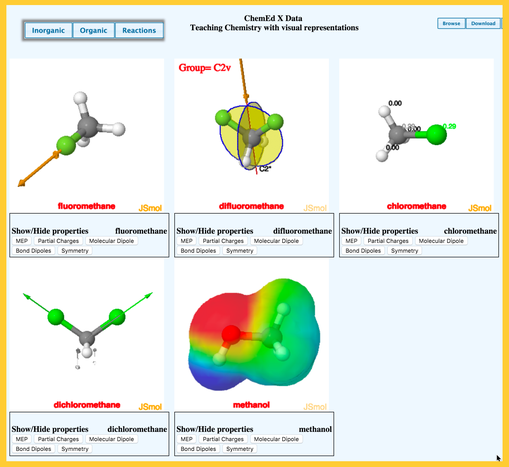
ChemEd X Data Website

http://chemdata.r.umn.edu

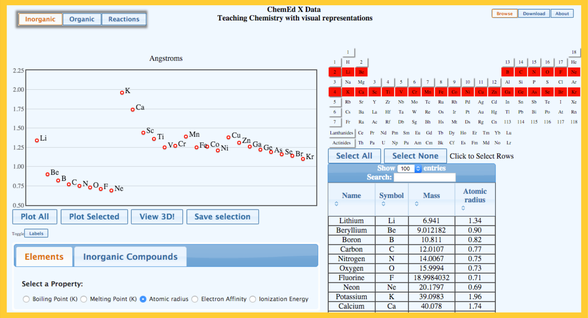
Flexible selection of compounds and their properties to discover trends in structure-property relationships: boiling and melting points, heat capacities, enthalpies of combustion, as a function of mass, shape, functional group…



Connecting it with molecular properties such as symmetry, charges and dipoles.



Navigate the periodic table to identify periodic trends or trends among inorganic compounds across a period or a group.
Example: lattice energy for LiCl, NaCl, KCl, RbCl…



Background

General Chemistry covers a wide variety of structure-property relationships that rely upon electronic, atomic, crystal or molecular structure. Often these submicroscopic factors come into conflict: What has a higher boiling point, methanol or hexane? What atom has a larger radius, Li or Mg? O or Cl?
A good strategy to address these "conflicting factors" is giving students experimental data at different points of the learning sequence. *ChemEd X Data* was designed to assist students as they create controlled experiments to test a relationship or as they investigate how different molecular factors affect a macroscopic property.

Implementation and Analysis

Using Sankey diagrams we can observe the flow of students performance as they move through the different types of questions.

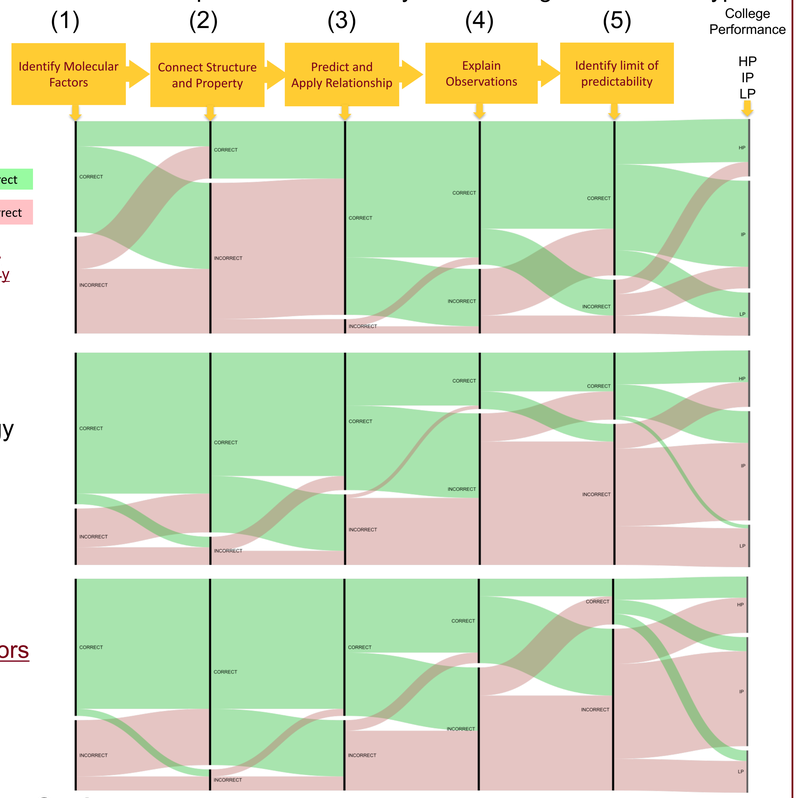
Activities using ChemEdXData site improve student performance

Boiling Point of molecular liquids
1) Identify functional groups and IMF
2) Create relationship: building CVS
3) Rank FG by BP
4) Explain mass or dipole: CH_xCl_y vs CH_xF_y
5) Limit of predict: Alkanes vs alcohols

Correct
Incorrect

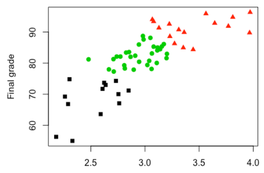
Ionic lattice energy of crystalline solids
1) Identify ion charge and trends in size
2) Effect of charge and size on bond energy
3) Apply: NaF vs CsI?
4) Does theory work if E(KCl)>E(NaBr)?
5) Limit of predict. NaCl vs KF

Periodic Table trends
1) Identify Z, shielding and orbital size
2) Use ChemEd X Data: connect radii/factors
3) Explain factors for regular PT trend
4) Explain factors for diagonal elements
5) Identify limit of predictability



College Performance: cluster GPA/Course Grade

HP: High performers
IP: Intermediate
LP: Low performers



Students perform very differently in CVS depending on different molecular factors

	% of all students who answered correctly	% of HP students who answered correctly	% of IP students who answered correctly	% of LP students who answered correctly	Final course grade average for students answering Correctly/Incorrectly
Create CVS branch effect	72.4%	81.3%	74.2%	46.2%	83.1/79.2; p = 0.12
Create CVS mass effect	46.6%	50.0%	48.4%	30.8%	83.1/81.1; p = 0.37
Create CVS IMF effect	27.6%	31.3%	32.3%	7.7%	85.8/80.6; p = 0.016

Conflicting factors and limit of predictability

In a first semester of General Chemistry there are several instances where the property of a substance is affected by more than one structural factor that come into conflict, making it impossible to predict. Data-first activities may help students identify these cases.

"Y": Property to be predicted	"X": Several factors that may come into conflict	Examples where theory in introductory courses does not predict an outcome
Boiling point of molecular liquids	Intermolecular forces, molecular shape and mass	Highest boiling point? Methanol vs Hexane
Periodic table trends: atomic size and ionization energy	Nuclear charge, electronic shielding and orbital size.	What element has a larger radius among diagonal elements? Li is bigger than Mg but O is smaller than Cl
Ionic lattice energy of a crystalline solid	Cation and anion size and their ionic charge	What compound has a higher ionic lattice energy, KF or NaCl?

Control of Variable Strategy (CVS)

Students provide evidence of a structure-property relationship by designing a controlled experiment: select a group of compounds that have all structural factors constant except the factor you want to test.
Example: *Select 4 compounds to show evidence of how the linear/branched chain may affect boiling points:*

Correct CVS: 273. 262. 309. 301.
Wrong CVS: 273. 355. 309. 341.

Summary

1) A unified approach to structure-property relationships allows the instructor to aim at specific skills of different cognitive levels throughout a General Chemistry semester.
2) *ChemEd X Data* facilitates the practice of some of these skills using data-first activities.
3) The type of questions that students have the most trouble with are: "Control of Variable Strategy" and "Identifying the limit of predictability"
4) Students can better identify the limit of predictability when using ChemEd X Data.
5) CVS exercises are only possible with data-first activities. Performance depends on the type of molecular factor being tested

Future directions

1) Interview students to investigate thought process
2) Technical developments:
   Bring open data to all chemistry curriculum, to all platforms http://github.com/xavierprat/chemEdData