Interdisciplinary energy: Can toy models from physics help students make sense of challenging chemical concepts?

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Outline

- Background
- Using a chemical context to achieve physics goals
- Exothermic reactions: A misconception?
- Exothermic reactions: Physics toy models
- A deeper analysis: The ontology of energy
- The physics in Gibbs free energy
  (no time for this – just a few comments)
- Some speculations

BACKGROUND

In the summer of 2010, HHMI offered four universities the opportunity to:

Develop prototype materials for biologists and pre-meds in

- *Chemistry (Purdue)*
- *Math (UMBC)*
- *Physics (UMCP)*
- *Capstone case study course (U of Miami)*

HHMI

nexus

NATIONAL EXPERIMENT
in Undergraduate Science Education

that would

- take an ***interdisciplinary perspective***
- be ***competency based***

The NEXUS/Physics team decided to change the goals of the course

- Traditional physics is "just physics": it ignores the needs and interests of bio students.
- We wanted to serve biology students and faculty by articulating with the biology curriculum
  - Provide support for difficult physics concepts that they will encounter in biology and chemistry classes.
- Use methods common in intro physics
  - Use simplified models to build understanding,
  - Build a sense of physical mechanism,
  - Develop coherences between things that initially seem contradictory, etc.

Changing the culture of the course

- Seek content and examples that have **authentic value for the biology curriculum.**
  - **Students** should see the course as helping them understand things are important for learning biology.
  - **Faculty** teaching upper division biology (and chemistry) should want physics as a pre-requisite.
- Assume this is a **2nd year** college course.
  - Biology, chemistry, and calculus are pre-requisites.
- Use **interactive engagement pedagogy**.
- A large **interdisciplinary team** was involved.

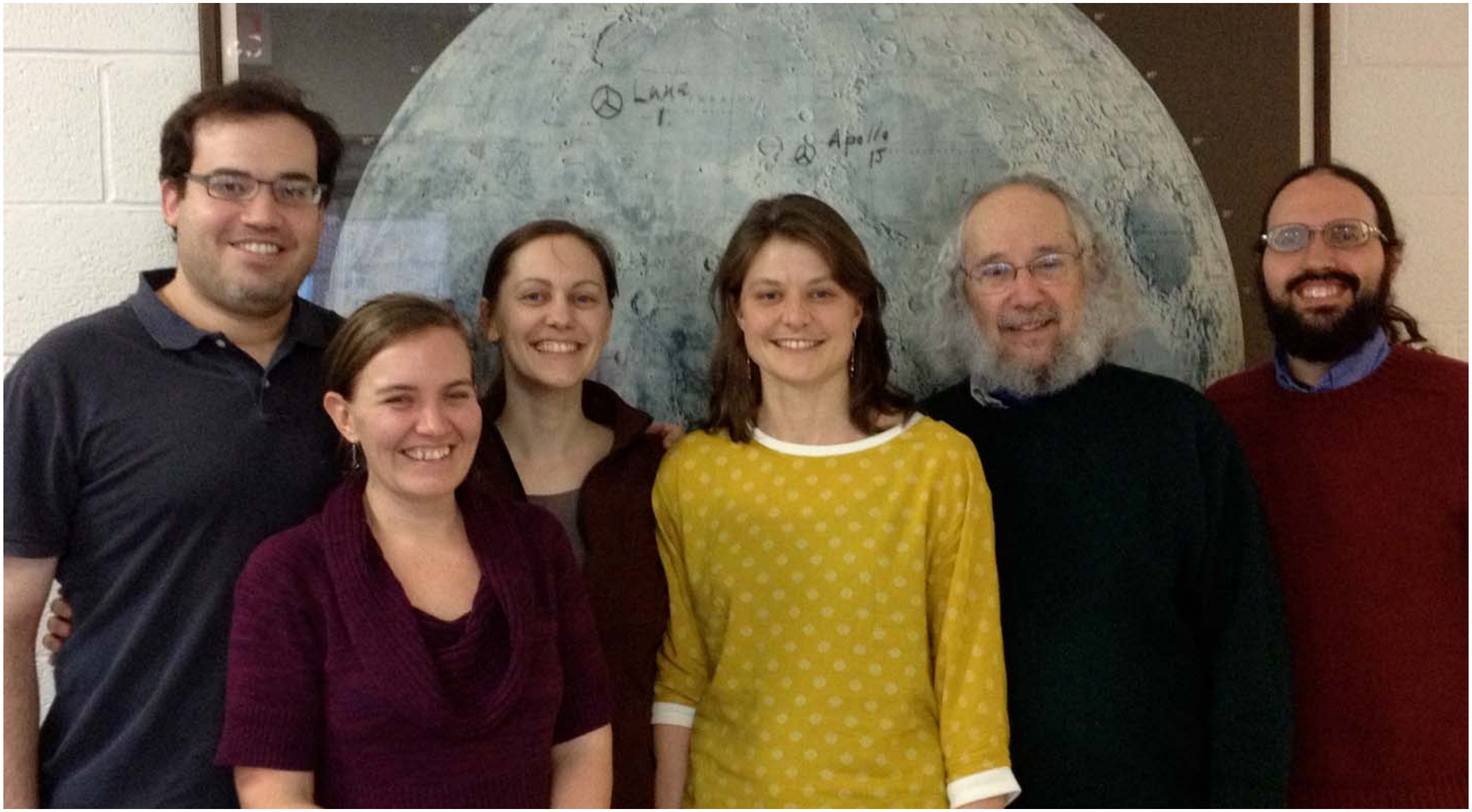
Redish et al., *Am. J. Phys* 82:5 (2014) 368-377

New interdisciplinary topics

- Focus on modeling and explicating assumptions.
- Do **micro and macro examples** throughout assuming students know about atoms and molecules.
- Include discussion of **chemical energy and reactions**
- Treat **random motion** as well as coherent. (Labs!)
- Carefully build the **basic statistical mechanics** support for thermodynamics (conceptually).
- Expand treatment of fluids and **physics in fluids**.

Dreyfus et al., *Am. J. Phys* 82:5 (2014) 403-411
Geller et al., *Am. J. Phys* 82:5 (2014) 394-402
Moore et al., *Am. J. Phys* 82:5 (2014) 387-393

The NEXUS/Physics Gang of Five + 1



Ben Geller (Bentropy) Vashti Sawtelle Chandra Turpen Julia Gouvea Joe Redish Ben Dreyfus (Benergy)

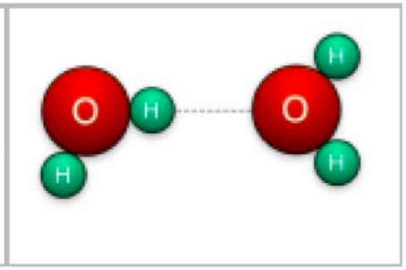
USING A CHEMICAL CONTEXT TO ACHIEVE PHYSICS GOALS

An example:
The physics side of a chemical situation

- Since we were putting in lots of new topics, we had to cut back on some traditional physics. What?
- One decision was to cut WAY BACK on inclined planes and projectile motion – topics that demonstrate basic physics principles but have little interest or relevance for life science students.
- But then how to help develop their skills with vectors?
- The answer: Bring electric forces to the first term as part of the introductory discussion of force. Calculate intermolecular forces in simple models.

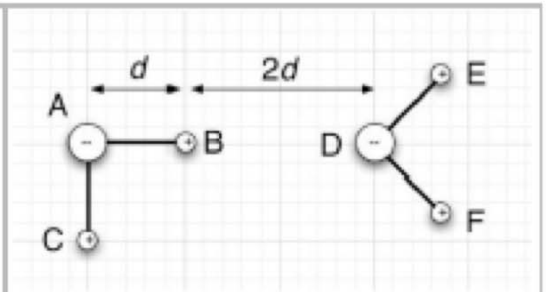
Hydrogen Bonding

We have seen that charged objects can attract neutral matter through the polarization of neutral matter – pushing the part of it that has the same charge slightly further away. At the molecular level, neutral molecules that have separated parts that are positive and negative can also attract one another by orienting properly. One example of this is *hydrogen bonding* of water molecules. This is the primary mechanism that creates surface tension in water (and a similar phenomenon plays a big role in a variety of biochemistry).

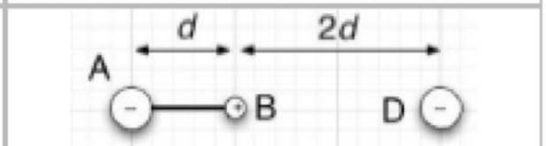


The hydrogens in a water molecule are positive (+e) and the oxygen is negative (-2e). Electric forces and the quantum sharing of electrons hold the whole thing together. We won't worry about this part inside the water molecule here but we will explore how the electric forces between water molecules properly arranged winds up being attractive.

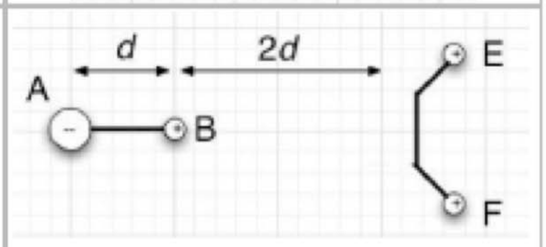
The angle between the hydrogen atoms in a water molecule is actually 104°, but in order to reduce your calculation for the purpose of this problem, we'll treat them as if they were a right angle – 90°. In a water-water hydrogen bond the separation between the hydrogen in one molecule and the oxygen in the other is about twice the distance between the hydrogen and the oxygen in its own molecule. Our simplified model is sketched in the figure at the right.



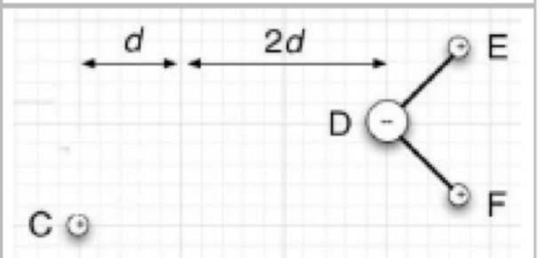
A. Consider the "backbone" of charges ABD. A and D repel, but B and D attract. Who wins? Does (AB) attract or repel D? By how much? Express your answer as a multiple of the force between two charges, *e*, at a distance *d*, $F_0 = k_e e^2/d^2$.



B. Now consider the force of (AB) on the "arms" of the other molecule – charges (EF). Is the force of (AB) on (EF) attractive or repulsive? In this case, you don't need to calculate the result exactly, but you have to be quantitative enough to be able to say convincingly which force is larger
(*Hint*: Reason quantitatively about distances but qualitatively about angles. Feel free to measure.)

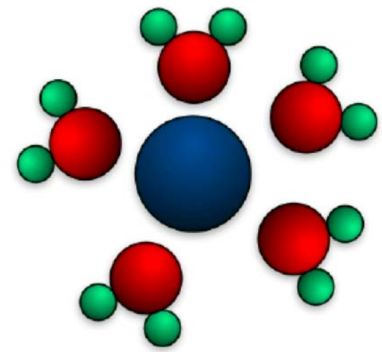


C. The only piece we've omitted is the force C exerts on (DEF). Say whether you think this will be significant in the overall attraction-repulsion balance and explain why you think so (briefly).

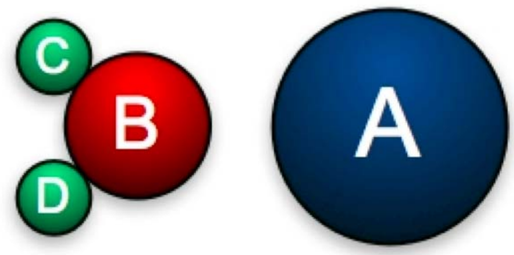


Water-coat Forces

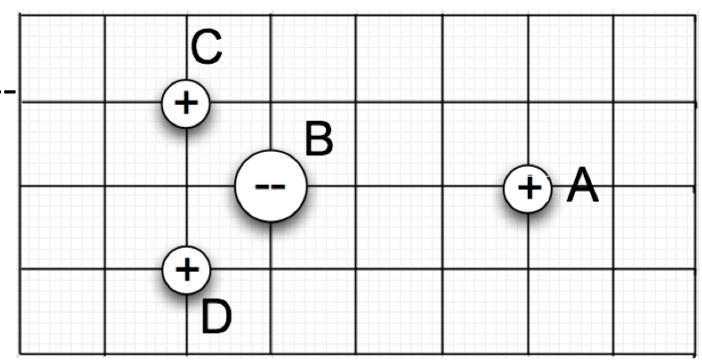
An important part of the functioning of a biological membrane is its ability to selectively pass either sodium ions (Na^+) or potassium ions (K^+) through membrane channels. Because these ions have the same charge (+e), the electric force exerted on them by the membrane will be similar. In addition, they are about the same size (R_{Na+}> ~ 0.12 nm, R_{K+}~ 0.15 nm) How can channels in the membrane distinguish them? One mechanism proposed to account for it is the suggestion that the ions attract water molecules that magnifies the effect of the small size difference between the ions.



To actually calculate the size of the ion's "water coat" is hard. (We would have to use quantum mechanics to include a repulsion force that keeps the atoms from getting too close to each other.) But we can get a first idea of what is happening by exploring the electric force between the ion and one water molecule as shown in the figure at the right.



To simplify the calculation, make a "simple physics model" -- take the ion and the two hydrogens as each having a charge +e, while the oxygen has a charge -2e. Treat each as point charges. ...

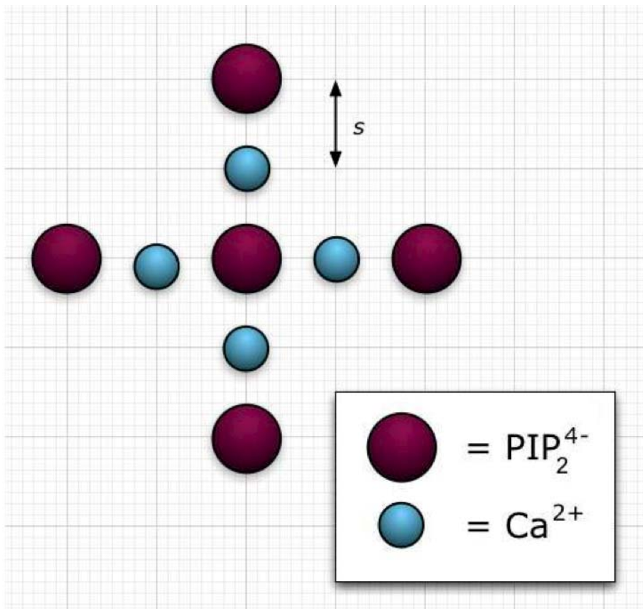


PIP_2 Cluster Stability

The phospholipid molecule PIP_2 (phosphatidylinositol 4,5-bisphosphate) is an important constituent of eukaryotic cell membranes. Its hydrophilic head group has a greater negative charge (typically -4e under physiological pH) than most of the other phospholipids present in eukaryotic cell membranes. PIP_2 makes up only a small fraction of the membrane (typically ~1% by mole fraction), but in spite of this low concentration, it is known to form clusters with multiple PIP_2 molecules that are thought to be important in cell signaling. It is an area of active research to understand the basis of this cluster formation.

Recent research* provides support for an electrostatic mechanism for this clustering, in which Ca^{2+} ions provide an attractive interaction holding together the PIP_2 molecules. The detailed structure of how Ca^{2+} ions and PIP_2 molecules are arranged in these clusters is not yet known. In this problem we consider a highly simplified model simply to give a feel for how these interactions might work.

In this problem we will explore whether the electric forces on the PIP_2 molecules in this model cluster tends to pull it together or blow it apart.



* Z. Li, et al.. Biophys. J., 97, 155-163 (2009).

The points

- The point of these problems is not to solve a specific problem in biochemistry. Our goals are more general and competency based.
    1. To help students develop and understanding of and a skill with manipulating vectors.
    2. To help students develop the idea that there is a *physical mechanism* underlying the properties and interactions of molecules.
    3. To help students develop the idea that many different results can follow from a few simple principles.

EXOTHERMIC REACTIONS: A MISCONCEPTION?

Example: Chemical bonding – A bridge through interdisciplinary reconciliation

- In introductory chemistry and biology classes, students learn about chemical reactions and the critical role of energy made available by molecular rearrangements.
- But students learn heuristics by rote that can feel contradictory to them and that they often don't know how to reconcile.

1. *It takes energy to break a chemical bond.*
2. *Breaking the bond in ATP is the "energy currency" providing energy for cellular metabolism.*

W. C. Galley, J. Chem. Ed., 81:4 (2004) 523-525.

M. Cooper and M. Klymkowsky, *CBE Life Sci Educ* 12:2 (2013) 306-312

A question from chemistry-education research

An O-P bond in ATP is referred to as a "high energy phosphate bond" because: (choose all correct answers)

✖ A. The bond is a particularly stable bond.

✔ B. The bond is a relatively weak bond.

✖ C. Breaking the bond releases a significant quantity of energy.

✔ D. A relatively small quantity of energy is required to break the bond.

	NEXUS	Galley
A	32%	41%
B	47%	31%
C	79%	87%
D	26%	7%

W. C. Galley, J. Chem. Ed., 81:4 (2004) 523-525.

We also thought this was a misconception – until a student convinced us otherwise.

Gregor gave B, C, & D on the quiz

- The bond is relatively weak and requires a small amount of energy to break
- Breaking the bond releases a large quantity of energy

Well, I mean, I put that when the bond's broken that's energy releasing. Even though I know, if I really think about it, that obviously that's not an energy-releasing mechanism. Because like, **you can't break a bond and release energy**, like you always need to put energy in, even if it's like a really small amount of energy to break a bond.

More than a “misconception”

Yeah, but like. I guess that's the difference between like how a **biologist** is trained to think, in like a larger context and how **physicists** just focus on sort of one little thing.

Whereas like, so I answered that it releases energy, but it releases energy because when an interaction with other molecules…in the end releases a lot of energy, but it does require like a really small input of energy to break that bond. **So I was thinking that larger context of this reaction releases energy.**

But wait, there's more!

I guess that's just the difference between physics and chemistry and biology. … It's just your scale.

Like, **physic[ists] really love to think about things in vacuums**, and like **without context**, in a lot of senses. So, you just think about like whatever small system you're— isolated system you're looking at, and **I guess chemist or biologists thinking about more of like an overall context**, that like wherever a reaction or process is happening, like that's important to what's going on.

Distinct disciplinary perspectives

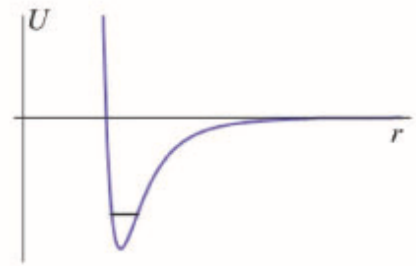
- Gregor is right! Physicists and biologists (and chemists) make different tacit assumptions.
- Physicists tend to isolate to focus on a particular physical phenomenon and mechanism.
- Biologists (and chemists) tend to assume the natural and universal context of life – a fluid environment (air and water taken for granted).
- We learned to not try to condemn one or other perspective as “wrong” but to be explicit and discuss the different ways different disciplines look at the same phenomenon – and why.

Midterm exam (Essay)

Two students discussing the process of ATP hydrolysis (ATP + H O → ADP + P) make the following comments:

Justin: The O-P bond in ATP is called a "high-energy bond" because the energy *released* when ATP is hydrolyzed is large. That released energy can be used to do useful things in the body that require energy, like making a muscle contract.

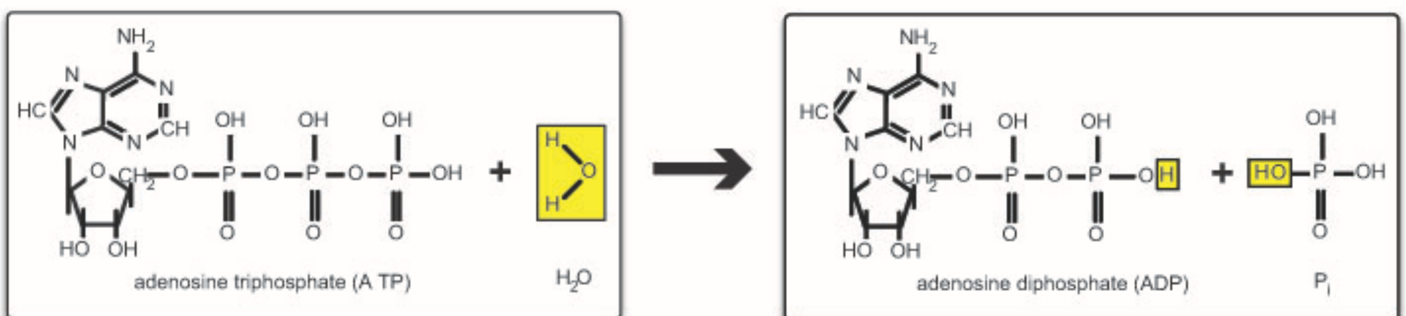
Kim: I though chemical bonds like the O-P bond in ATP could be modeled by a potential energy curve like this (she draws the picture at the right), where *r* is the distance between the O and the P. If that's the case, then breaking the O-P bond in ATP would require me to*input* energy. I might not have to input *much* energy to break it, if that O-P happens to be a weak bond, but shouldn't I have to input at least *some* energy?



How did Kim infer from the PE graph that breaking the O-P bond requires an input of energy? Who's right? Or can you reconcile their statements?

(The chemical structures of this process are given below if you find that useful)

Note: This is an essay question. Your answer will be judged not solely on its correctness, but for its depth, coherence, and clarity.

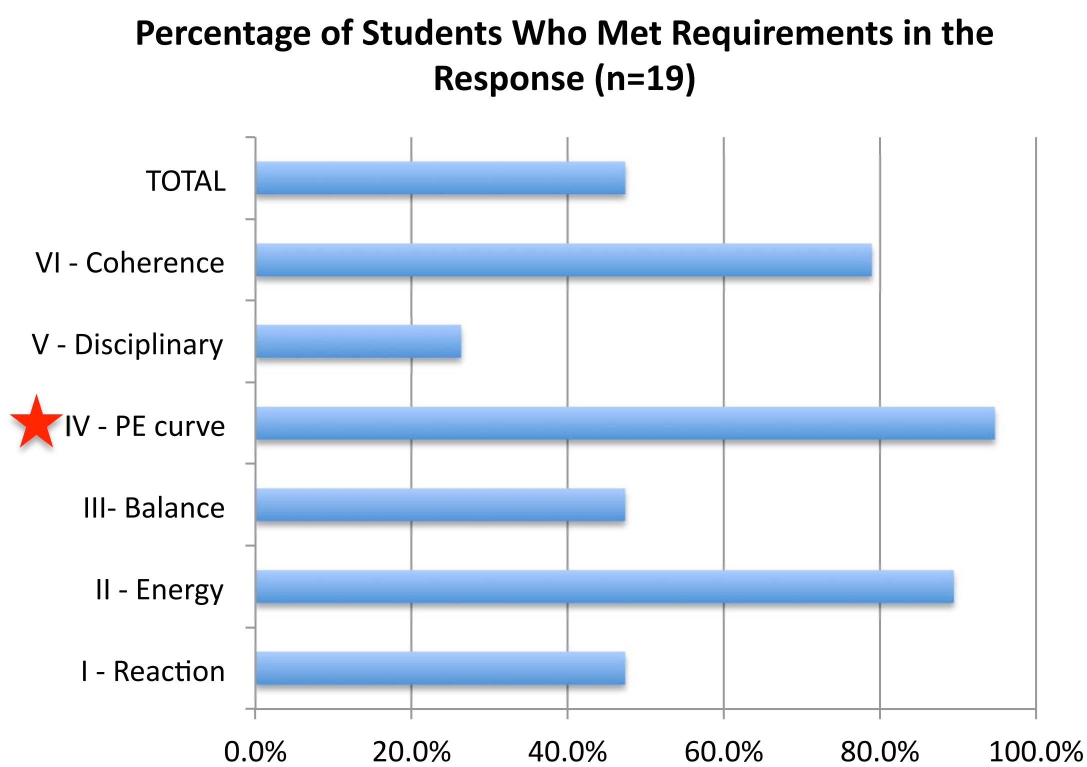


Rubric Analysis of ATP Question

I) 47% students recognized bonds are both broken and formed

II) 90% of students connected breaking and forming of bonds to the *U* vs *r* curve

III) 47% of students recognized that the energy of forming new bonds outweighed the energy of breaking the O-P

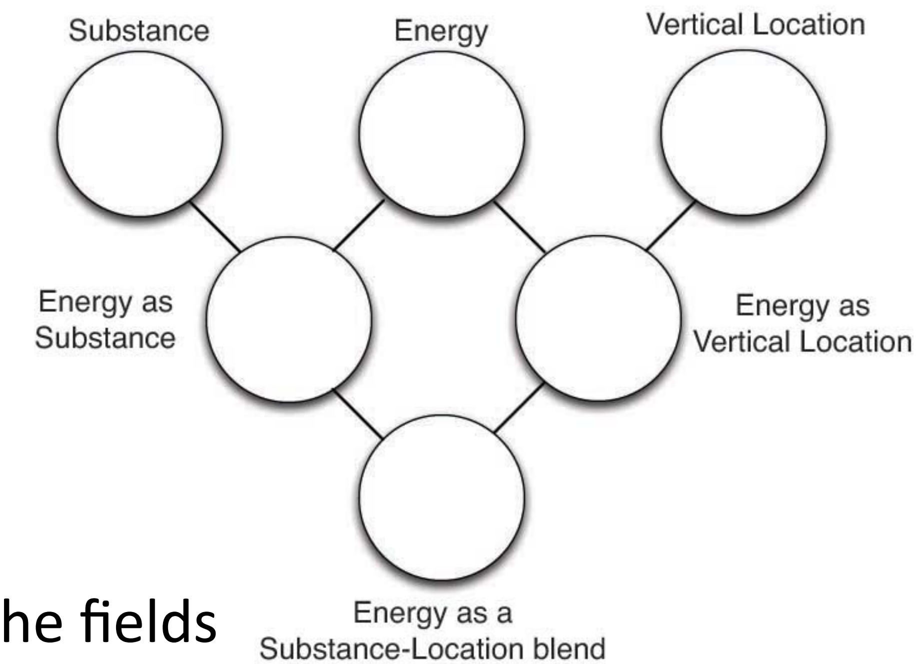


Rubric at:
http://umdberg.pbworks.com/w/page/52816586/ATP%20Exam%201:%20Rubric

A DEEPER ANALYSIS: THE ONTOLOGY OF ENERGY

Making sense of energy

Since we don't have a direct sensory measure of the concept of energy we have to build it as we do other abstract concepts: by metaphor, analogy, and blending of other concepts that eventually rest in direct physical experience and perception.

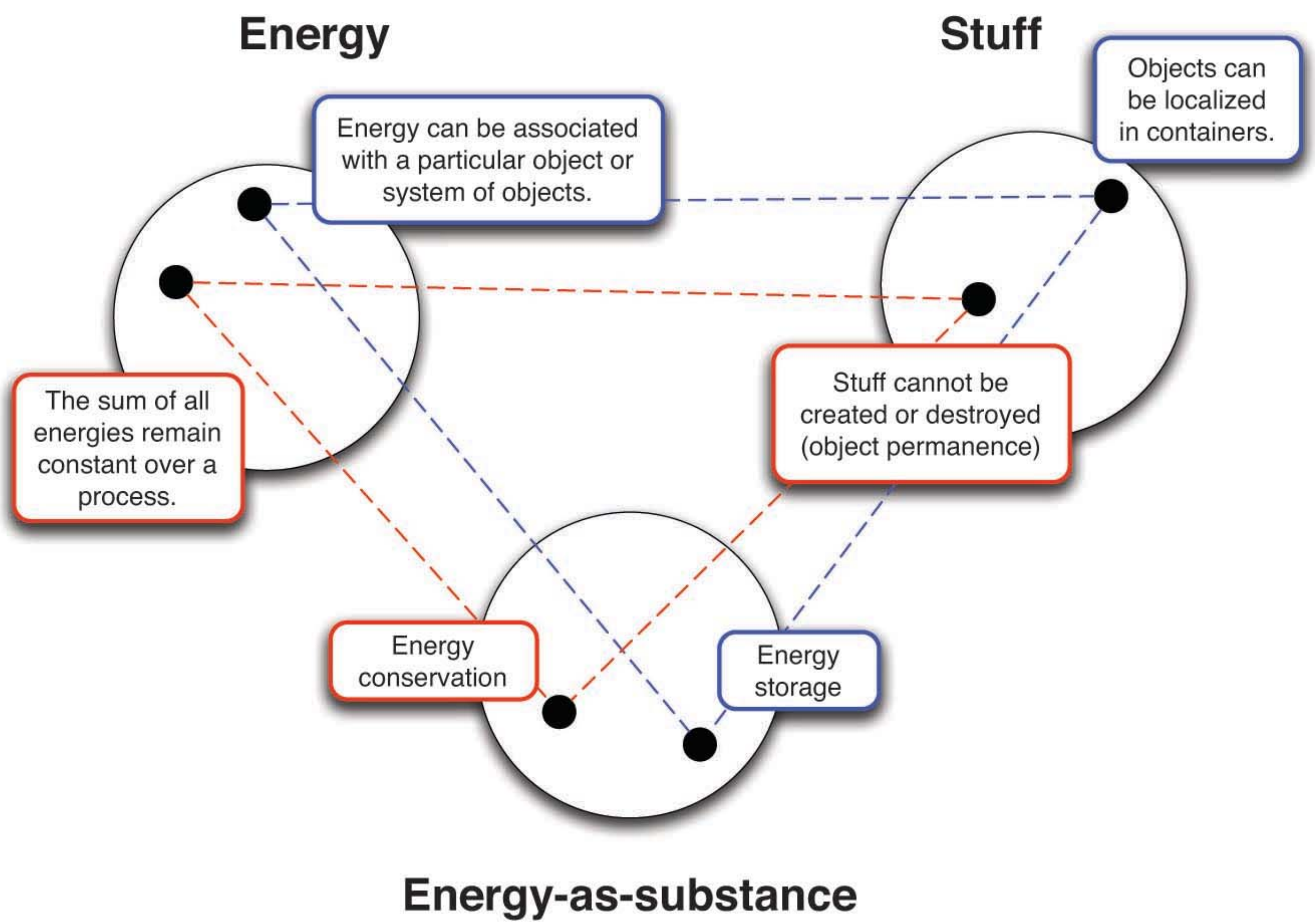


This is a well studied approach in the fields of linguistics, pragmatics, and semantics.

G. Lakoff & M. Johnson, *Metaphors we Live By* (U. Chicago Press, 2003)
G. Fauconnier & M. Turner, *The Way We Think: Conceptual Blending and the Minds Hidden Complexities* (Basic Books 2003)
J. Füster, *Cortex and Mind: Unifying Cognition* (Oxford U. Press, 2003)

A professional physicist's view of energy is complex and blends multiple metaphors.

Energy as a Substance metaphor as a conceptual blend



Energy as a Vertical Location metaphor as a conceptual blend

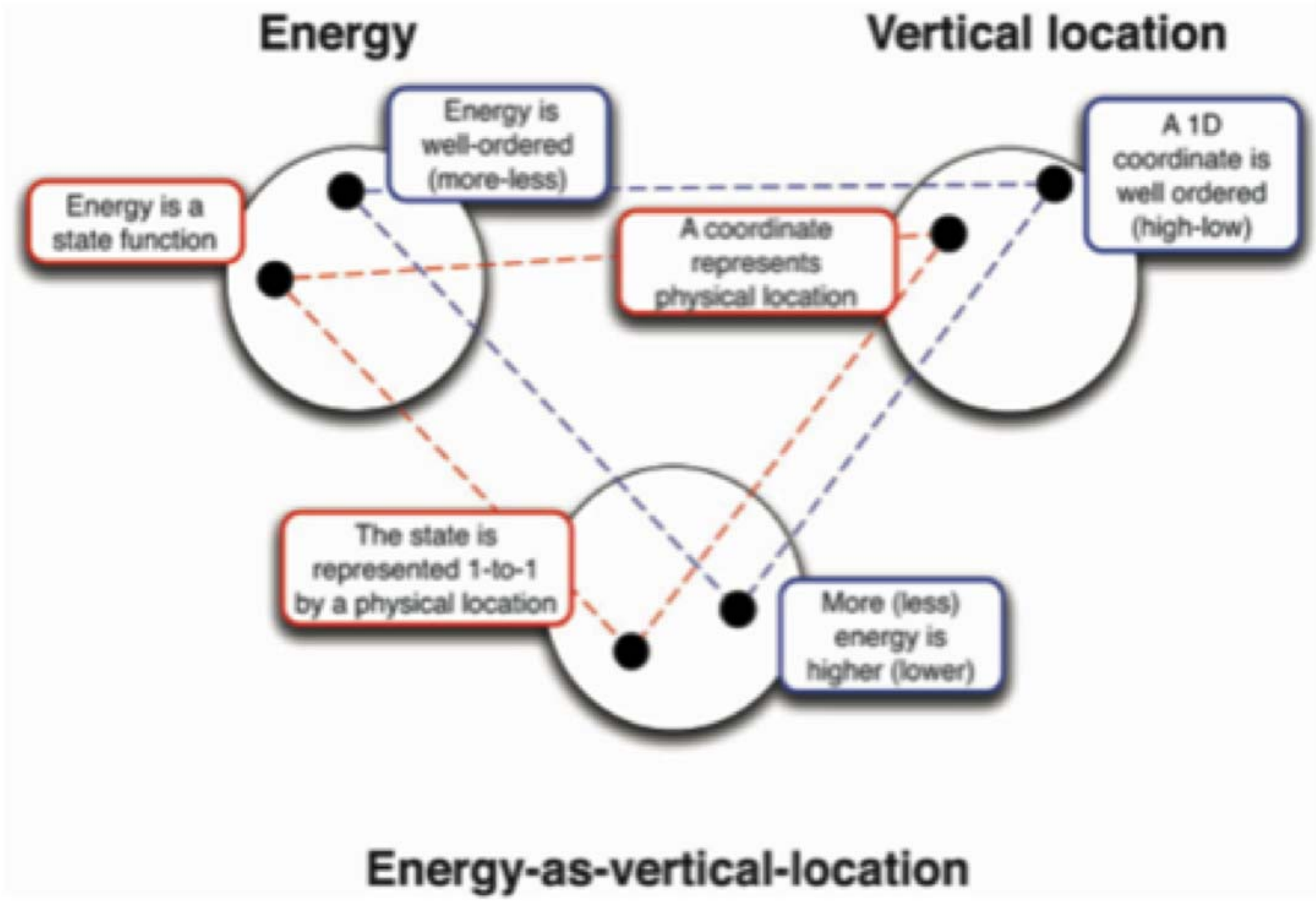
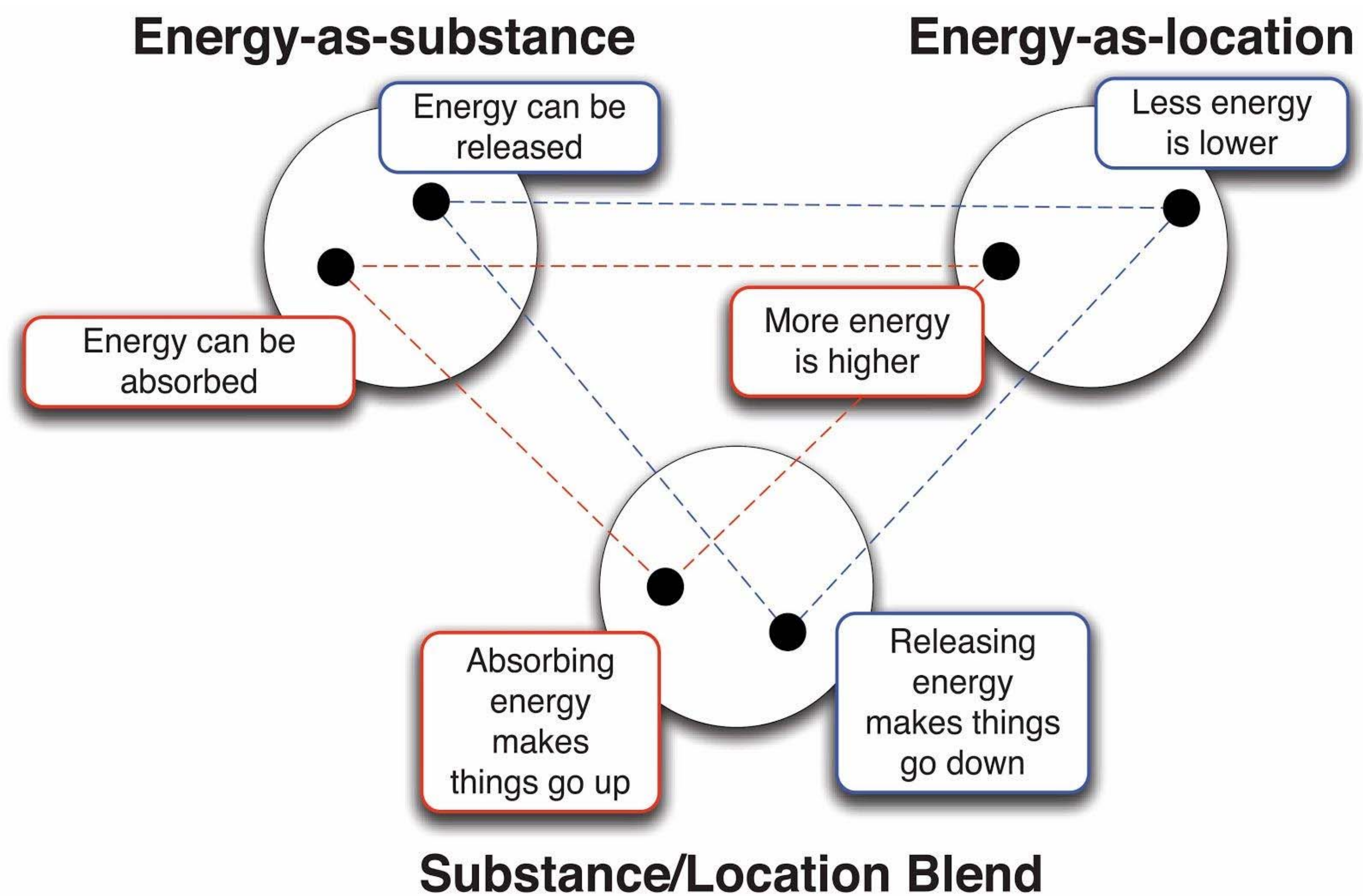


Figure 3. The energy-as-vertical-location blend.

Blending the substance and location metaphors



Using the blended space

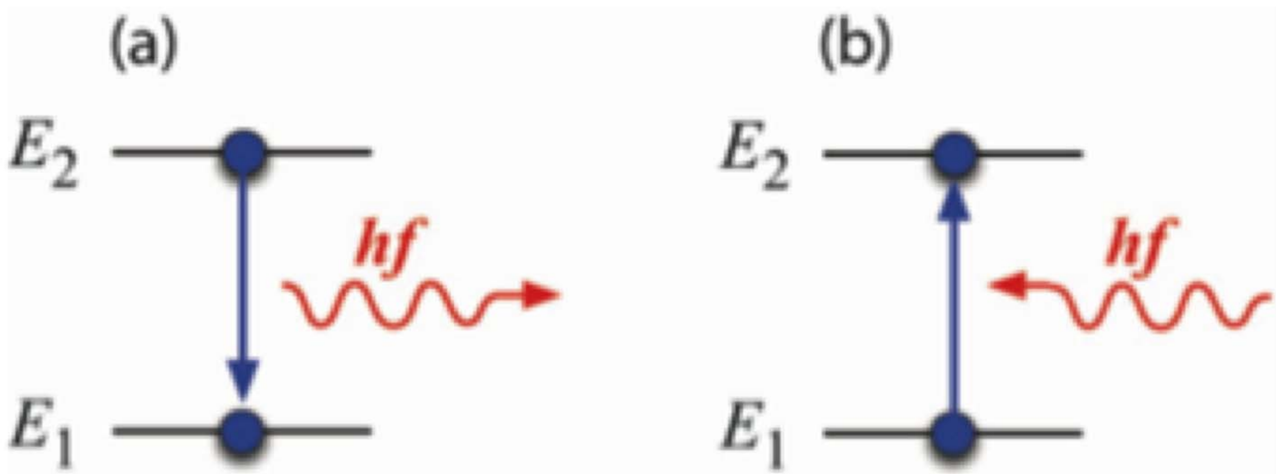


Figure 5. Representation of absorption and emission of energy from the a quantum system. (Wikipedia, 2014).

We have evidence that this is a blend (not switching) and that both students and expert faculty can use it.

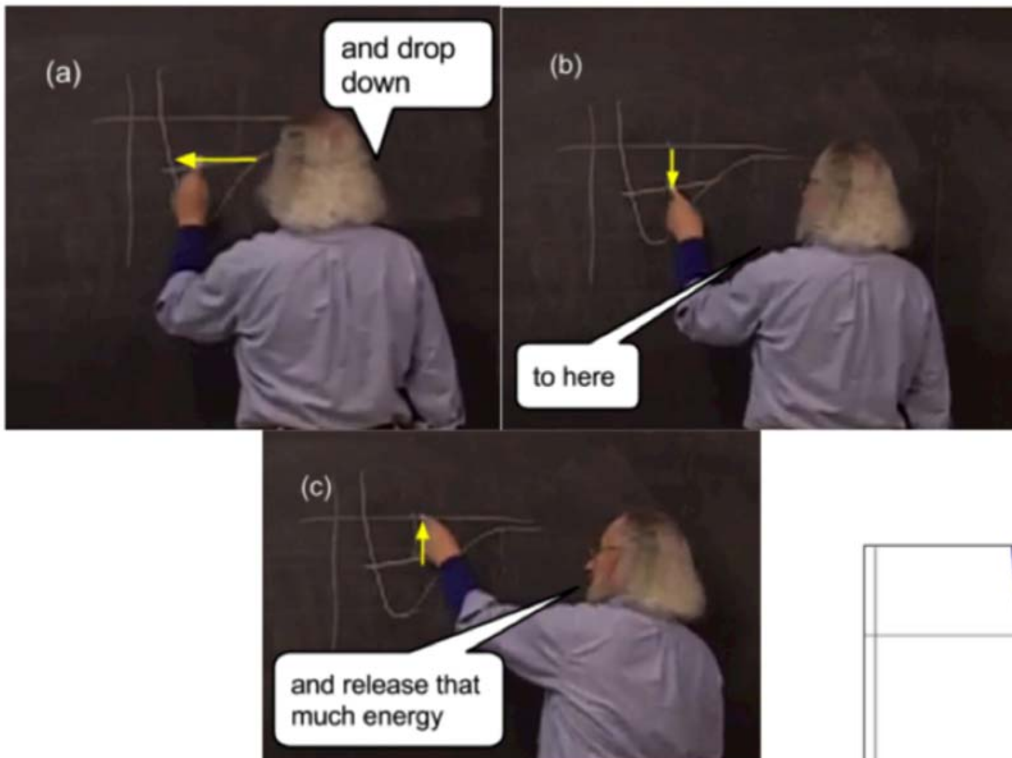


Figure 9. Prof. Farnsworth draws (a) a horizontal line about halfway down the well, (b) a double-tipped vertical arrow from the top of the well to that line, and (c) a ver from the horizontal line in the middle of the well to the top of the well. (Note that t arrows added to the figure represent his hand motion as he produces the inscription

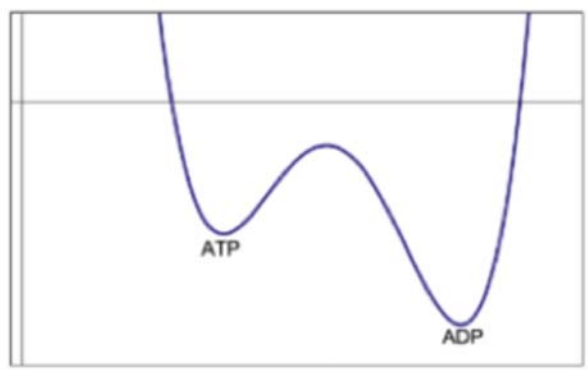


Figure 12. The energy diagram that Betsy draws, representing ATP and ADP on the same graph

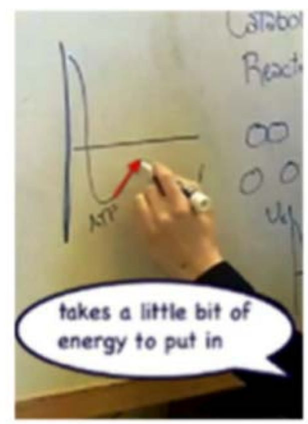
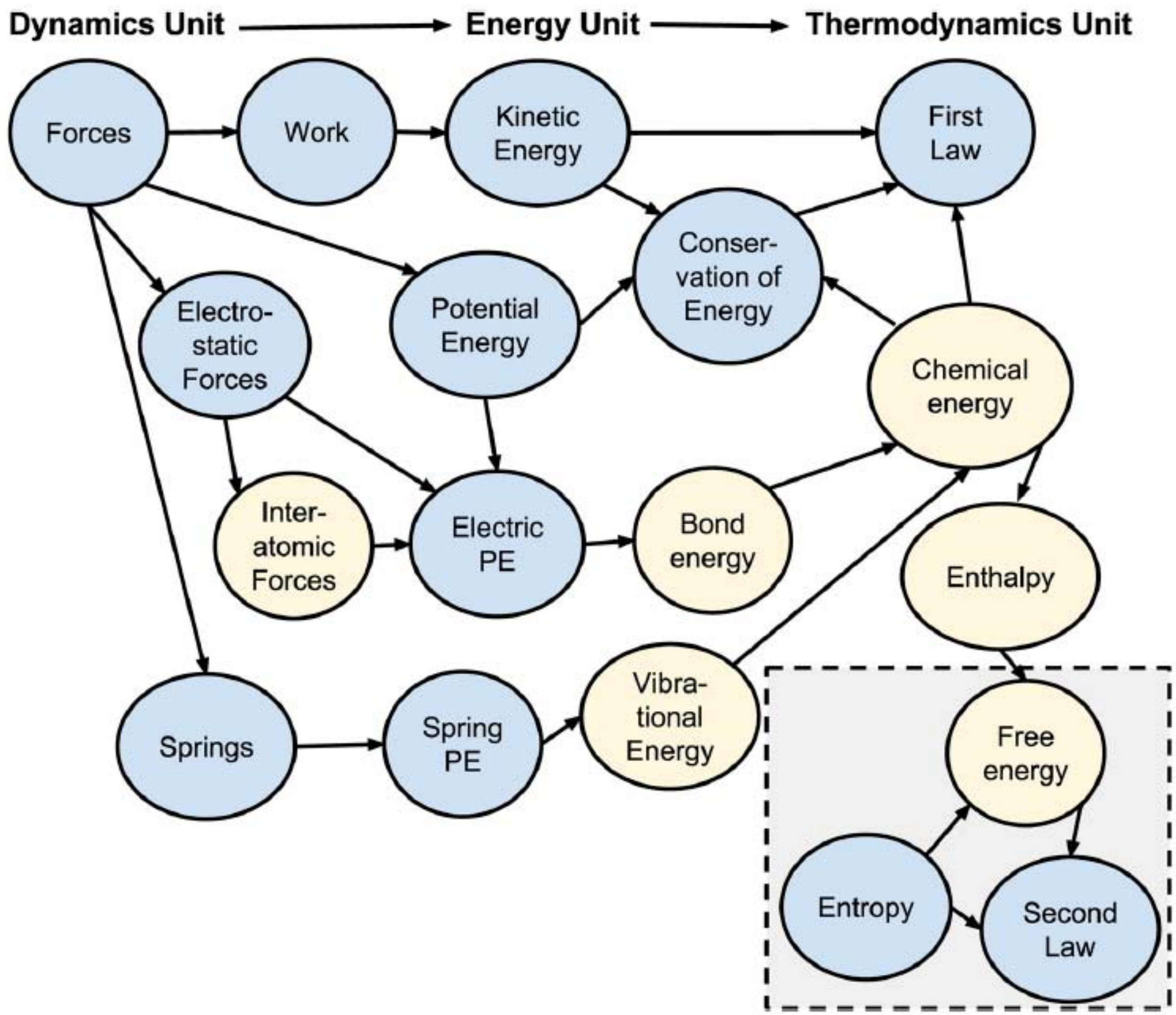


Figure 13. Betsy traces up along graph from ATP well and then back down into deeper well (labeled as ADP)

EXOTHERMIC REACTIONS: PHYSICS TOY MODELS

The NEXUS/Physics Chemical Energy Thread



Example 2: Chemical bonding

- In intro chem and bio classes, students learn about chemical reactions and the critical role of energy made available by molecular rearrangements.
- But students often learn heuristics by rote. These may feel contradictory to them and they may not know how to reconcile.

    1. *It takes energy to break a chemical bond.*
    2. *Breaking the bond in ATP is the "energy currency" of cellular metabolism.*

W. C. Galley, J. Chem. Ed., 81:4 (2004) 523-525.

How does the ontology of energy help create the problem?

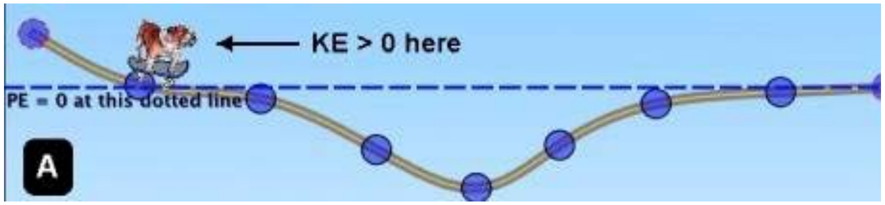
- If students think of energy only as "stuff" then they have a lot of trouble with "negative energy" associated with a bond.
- The difference between "binding energy" (a negative quantity) and "bond energy" (a positive quantity) confuses students if they are thinking of energy as "stuff."

Many students infer a “piñata” model of a chemical bond.

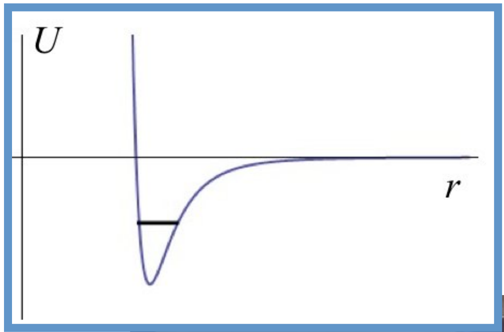
"But like the way that I was thinking of it, I don't know why, but whenever chemistry taught us like exothermic, endothermic, like what she said, I always imagined like the breaking of the bonds has like these little [energy] molecules that float out, but like I know it’s wrong. But that's just how I pictured it from the beginning."

Can physics help?

- Build a coherent story using toy models
  - Bulldog on a skateboard



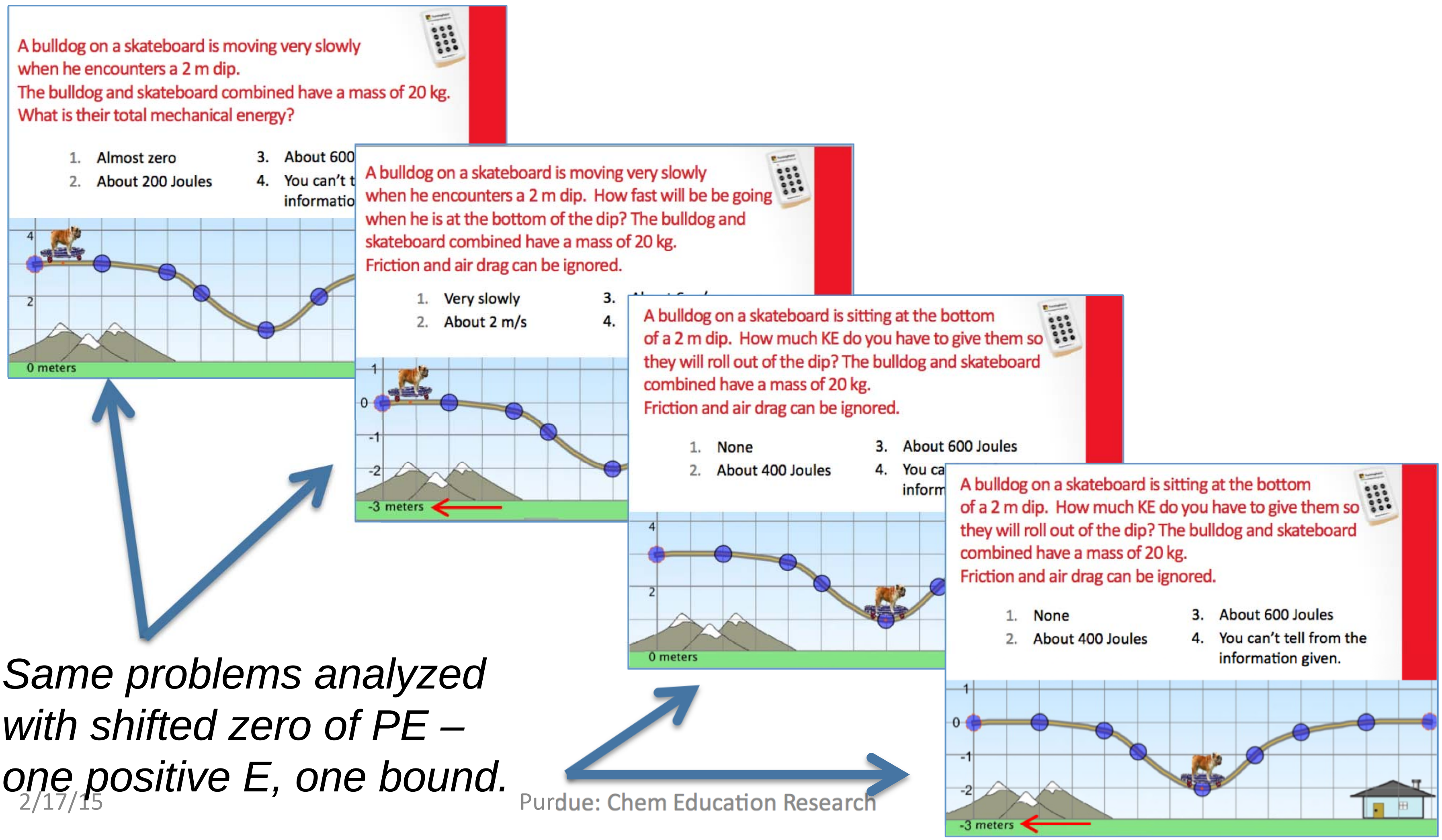
  - Atomic interactions and binding



  - Reactions in which bonds are first broken and then stronger ones formed (the Gauss gun)

This set of instructional materials won an award from the AAMC MedEd Portal

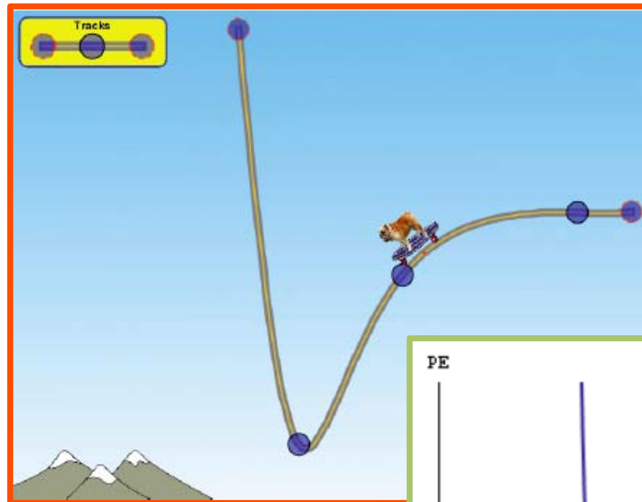
A series of clicker questions (PhET based) helps students get comfortable with negative PE and with the concept of binding energy.

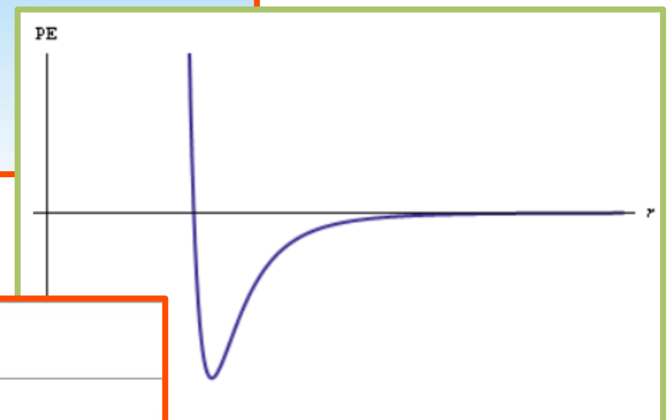


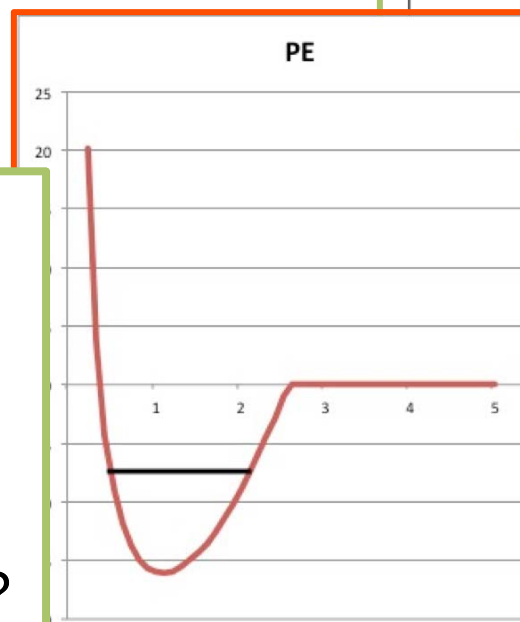
Same problems analyzed with shifted zero of PE – one positive E, one bound.

Bound states HW problem

The skateboarder is just an analogy for the cases we are interested in -- interacting atoms.

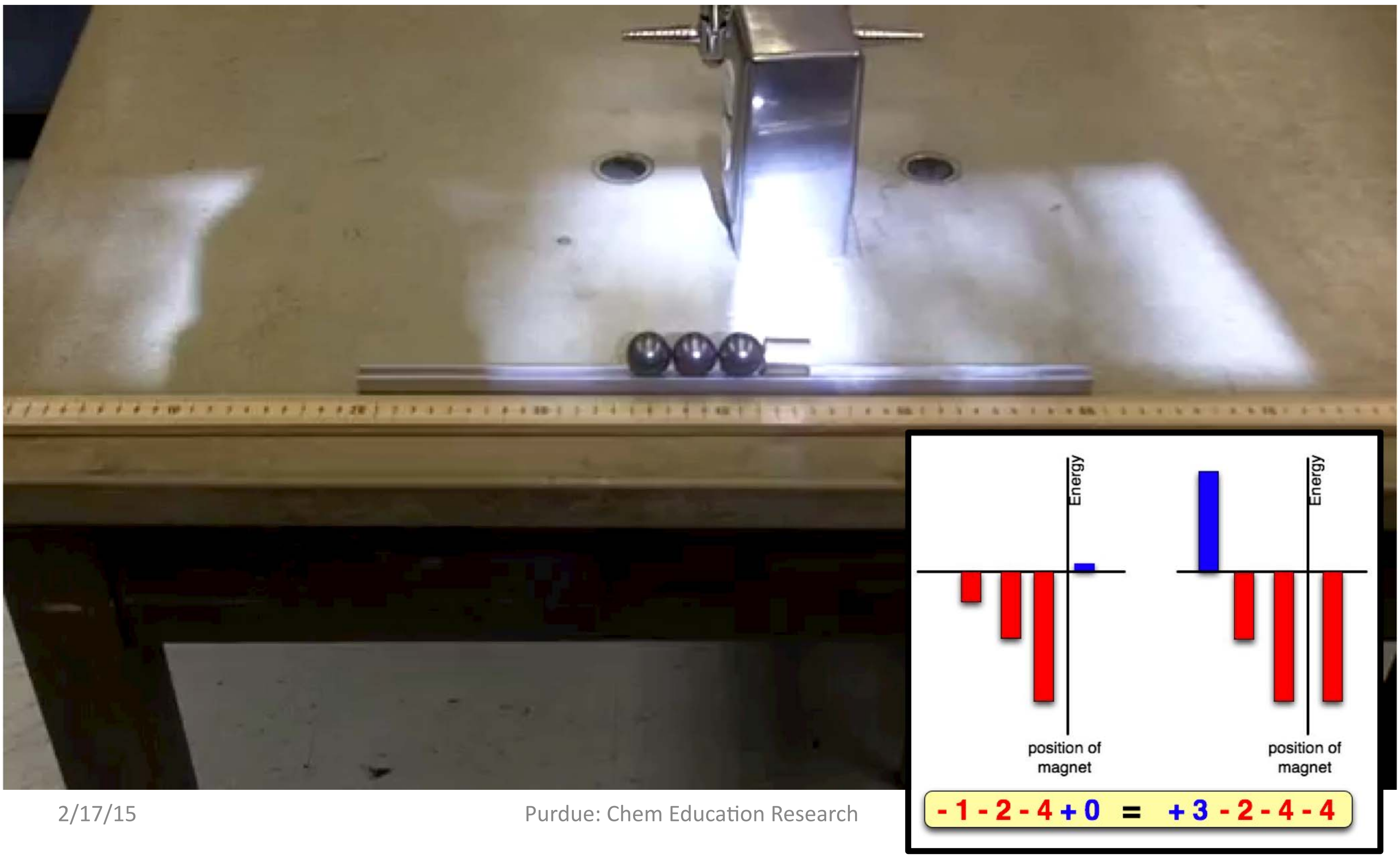




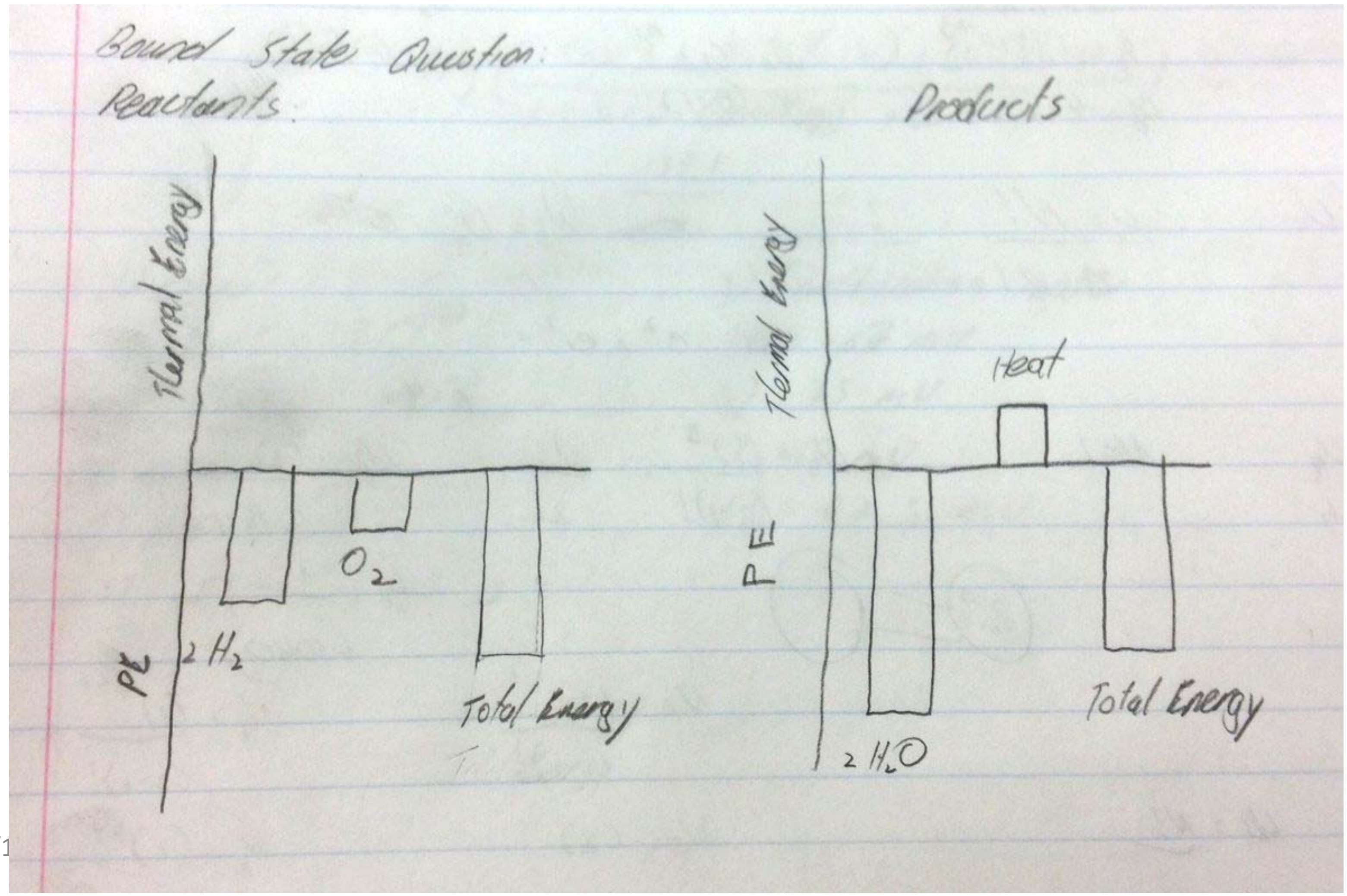


If the atoms have an energy of -7.5 units as shown by the solid line in the figure, would you have to put in energy to separate the atoms or by separating them would you gain energy? How much? Explain why you think so.

The Gauss Gun: A classical analog of an exothermic reaction



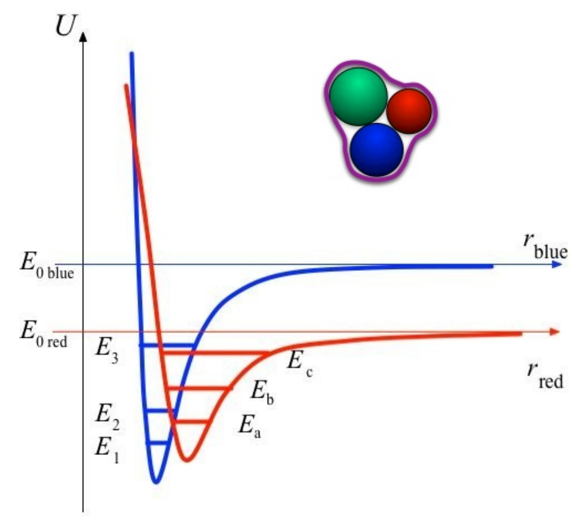
Student drawing from a HW on the reaction $H_2 + O_2 \rightarrow 2H_2O$



Final exam (MC)

The figure at the right depicts a situation in a chemical reaction complex . We model the combined system as consisting of three parts, shown red, green, and blue. Each part can be pulled away from the remaining pair or vibrate against them.

Two potential energy curves are shown: one in blue that shows what happens to the potential energy as the blue part is pulled away from the red-green pair, one in red that shows what happens to the potential energy as the red part is pulled away from the blue-green pair.



6.2 (5 pts) Which part takes less energy to break off from the molecule, blue or red?

a. The blue part.
b. The red part.
c. They will each take the same energy to remove.
d. You can't tell from the information given.

	6.2
a	5%
b	95%

References

- Chemical energy in an introductory physics course for the life sciences, B. W. Dreyfus, B. D. Geller, J. Gouvea, V. Sawtelle, C. Turpen, & E. F. Redish, *Am. J. Phys. 82:*5 (2013) 403-411.
- Students' reasoning about high energy bonds and ATP: A vision of interdisciplinary education, B. W. Dreyfus, B. D. Geller, J. Gouvea, V. Sawtelle, C. Turpen, & E. F. Redish, *Phys. Rev. ST Physics Education Research 10* (2014) 010115, 15 pages.
- Ontological metaphors for negative energy in an interdisciplinary context, B. W. Dreyfus, B. D. Geller, J. Gouvea, V. Sawtelle, C. Turpen, & E. F. Redish, *Phys. Rev. ST Physics Education Research 10* (2014) 020108, 11 pp.
- Applying Conceptual Blending to Model Coordinated Use of Multiple Ontological Metaphors, B. W. Dreyfus, A. Gupta, and E. F. Redish*, Int. J. Sci. Ed*. (2015) in press.