Carbon TIME Content Simplifications

There are a number of places where our learning progression research or other considerations lead us to build *Carbon TIME* materials around simplified models of the systems and processes that the students are studying. This is a standard scientific practice—all models involve some kinds of simplifications.

General criteria for appropriate simplifications

To quote the statistician G. E. P. Box (1979), "All models are wrong but some are useful." Scientists customarily use an array of models to understand the systems that they study, understanding that every model is "wrong" in the sense that it includes simplifying assumptions and produces appropriate predictions and explanations for a limited range of phenomena. Thus good scientists do not know "correct" models; instead, they are able to choose models that are useful for particular purposes and explain the limitations of those models.

Curriculum developers face problems similar to scientists, but with an added complication: Models that scientists might choose as the most useful in a certain situation may be incomprehensible to students. In particular, models that are scientifically simple and elegant often rely on scientific theories (e.g., atomic-molecular theory) that students may not be prepared to fully understand. Therefore in curriculum development we need simplified models and principles that meet four criteria:

1. *Comprehensibility:* They are comprehensible to students, as indicated by our learning progression research. In particular, the students we are writing for:
    - Generally know some facts about atoms and molecules, but have not mastered functional atomic-molecular models (Mohan, Chen, & Anderson, 2009).
    - Think of energy as something that causes events to happen or enables organisms to act (e.g., "I have a lot of energy after a good night's sleep." "Five-hour Energy Drink gives you energy." Jin & Anderson, 2012).
2. *Efficiency:* Understanding is achievable within reasonable constraints on instructional time.
3. *Consistency*: They can be used consistently across the range of systems and processes that we are studying (in the case of *Carbon TIME*, carbon-transforming processes in biogeochemical and technological systems) and across scales:
    - Atomic-molecular, focusing on atoms, molecules, and chemical bonds but NOT on subatomic particles (a decision made for reasons of efficiency; to explain structure of atoms and molecules using subatomic particles would take too much time)
    - Macroscopic, focusing on systems, materials, and manifestations of energy (chemical, heat, light, work/motion) that are visible to students in the world around them.

   - Large-scale, focusing on energy flow in ecosystems and human technological systems

4. *Productivity for future learning:* They position students to understand more sophisticated models in their future learning.

Three Question framework

The *Carbon TIME* curriculum is organized around the framework of the Three Questions (Table 1 below), so I'll use this table to organize an initial list of simplifications.

Table 1: The Three Questions

Question	Rules to Follow	Connecting Atoms to Evidence
The Location and Movement Question: Where are atoms moving? Where are atoms moving from? Where are atoms going to?	**Atoms last forever** in combustion and living systems All materials (solids, liquids, and gases) are made of atoms	When materials change mass, atoms are moving When materials move, atoms are moving
The Carbon Question: What is happening to carbon atoms? What molecules are carbon atoms in before the process? How are the atoms rearranged into new molecules?	Carbon atoms are bound to other atoms in molecules **Atoms can be rearranged to make new molecules**	The air has carbon atoms in CO_2 Organic materials are made of molecules with carbon atoms • Foods • Fuels • Living and dead plants and animals
The Energy Question: What is happening to chemical energy? What forms of energy are involved? How is energy changing from one form to another?	**Energy lasts forever** in combustion and living systems C-C and C-H bonds have more stored chemical energy than C-O and H-O bonds	We can observe indicators of different forms of energy • Organic materials with chemical energy • Light energy • Heat energy • Work or motion energy

Simplifications organized according to the Three Questions

1. The Movement Question
    a. Atoms last forever: We limit this claim to the processes we are studying (combustion and living systems), but we do not discuss nuclear changes
    b. Movement of materials in plants: When students model movement of materials in plants, we have them moving glucose monomers rather than sucrose molecules from leaves to other parts of the plant
    c. Movement of materials in animals and decomposers: When students model movement of materials through the blood, we have them moving monomers—glycerol, fatty acids, amino acids, glucose—through the blood or mycelium
2. The Carbon Question
    a. We strictly separate matter from energy in accounting for chemical changes, not mentioning matter-energy equivalency
    b. We trace individual atoms through processes while ignoring the roles of pools of atoms in intermediate states (for example, we model all 6 H atoms in a molecule of ethanol ending up in exactly 3 H_2O molecules, something that is unlikely to happen in a real flame.
    c. In modeling cellular respiration, we have students use a standard but simplified formula for the overall chemical change:

       $$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ CO_2 + 6\ H_2O$$

       This incorrectly suggests that some of the oxygen atoms in O_2 end up in CO_2, which is not actually the case. A more accurate formula to represent the multi-step process would be as follows:

       $$C_6H_{12}O_6 + 6\ \mathbf{O}_2 + 6\ H_2O \rightarrow 6\ CO_2 + 12\ H_2\mathbf{O}$$

       Where atmospheric oxygen acts as the electron receptor at the end of the electron transport chain and all ends up in H_2O
    d. We make a similar simplification in modeling photosynthesis, incorrectly suggesting that some of the oxygen in CO_2 is released into the atmosphere as O_2, rather than showing all of the released O_2 coming from H_2O.
    e. We simplify the processes of biosynthesis, suggesting generally that biosynthesis involves making polymers from monomers. We include ideas that plants can make other monomers from glucose and soil minerals, and that animals can make fats from sugars. We do not mention many other kinds of atoms and molecules and biosynthetic pathways.
3. The Energy Question
    a. Energy lasts forever: We do not discuss the equivalency of matter and energy.
    b. We restrict students modeling activities to four different forms of energy, each of which is simplified in some way:

i. Light energy: we refer to light energy as in input to photosynthesis, but do not discuss the idea that infrared radiation going into space is also part of the electromagnetic spectrum

ii. Heat energy: we do not distinguish between heat as an energy transfer process and thermal energy. Thus we do not address, for example, the different forms of energy associated with different heat transfer processes (conduction, convection, radiation).

iii. Work or motion energy: we do not distinguish between work as an energy transfer process and kinetic energy; we also do not clearly define “work.”

iv. Chemical energy: we describe chemical energy as “stored” in high-energy (C-H and C-C) bonds in organic molecules rather than as a more general characteristic of systems that also contain oxygen—and chemical energy as released when C-C and C-H bonds are replaced with lower energy C-O and H-O bonds in combustion or cellular respiration. We do not mention electrons or energy states of electrons.

Issues in developing a consistent model for chemical energy

The energy story in *Carbon TIME* units is essentially a story of chemical energy. This is the new idea that students MUST understand in order to learn meaningfully from the units. So developing a model of chemical energy that fits the criteria above: comprehensibility, efficiency, consistency, and productivity for future learning, is essential.

On the following pages I will try to use these criteria to evaluate a number of possible candidates for such a model, ending with an explanation of the model we have chosen.

Looking at the NRC model(s)

We want the *Carbon TIME* framework to be aligned with the *Next Generation Science Standards,* so the NRC *Framework* is an obvious place to look for guidance. Energy is addressed at multiple places in the *Framework*, particularly in the sections on crosscutting concepts and disciplinary core ideas in physical science.

Energy as a crosscutting concept: The NRC *Framework* describes energy in the section on energy and matter as a crosscutting concept (pages 94-5) that has essentially a 19th-century definition of energy. Energy is:

- Different from matter
- Without mass

- Conserved in physical and chemical processes, and therefore traceable through these processes.

This description clearly makes compromises for the sake of simplicity and parsimony, ignoring ways in which relativity and quantum mechanics indicate that each of the three assertions about energy above is merely an approximation that ignores deeper connections between matter and energy and can be used within a limited range of temporal and spatial scales.

I like this description a lot, though. It meets the criteria above of simplicity, parsimony, and consistence, and the three bullets above capture the essential principles of an energy model that is scientifically meaningful. Whatever model we use for *Carbon TIME must* have these characteristics. But a model that can be used to analyze carbon-transforming processes must go beyond these general principles; we need specific rules for applying it to the systems and processes we are studying.

Energy as a disciplinary core idea. The NRC *Framework* describes a more detailed model of energy in the section on energy as a core disciplinary idea. Here are some key aspects of that description:

> At the macroscopic scale, energy manifests itself in multiple phenomena, such as motion, light, sound, electrical and magnetic fields, and thermal energy. Historically, different units were introduced for the energy present in these different phenomena, and it took some time before the relationships among them were recognized. Energy is best understood at the microscopic scale, at which it can be modeled as either motions of particles or as stored in force fields (electric, magnetic, gravitational) that mediate interactions between particles. (p. 121).
>
> The idea that there are different forms of energy, such as thermal energy, mechanical energy, and chemical energy, is misleading, as it implies that the nature of the energy in each of these manifestations is distinct when in fact they all are ultimately, at the atomic scale, some mixture of kinetic energy, stored energy, and radiation. (p. 122)

This description is much more specific than the description in the crosscutting concepts section, and it meets the criterion of consistency above. Cooper and Klymkowsky (in press) argue convincingly that it is appropriate for college-level courses and superior to the current treatments of energy in those courses. Unfortunately, it does not meet the criteria of comprehensibility and efficiency for the middle school and high school students for whom *Carbon TIME* is written. In particular, we cannot expect middle school and high school students to understand carbon-transforming processes on a subatomic scale. For evidence to support this assertion, see Jin & Anderson (2012). We need a simpler model of energy that still conforms with the basic principles described in the section on energy as a crosscutting concept (the three bullets above).

Looking at scientific models

So for *Carbon TIME* we can't just pull a model of energy from the NRC Framework. We need a way to deal with energy without using detailed subatomic models of matter. In deciding what form this energy model should take, there are several scientific models that we can consider. Each is accepted as an approach to accounting for energy on a macroscopic or ecosystem scale. Each also involves simplifications of the NRC disciplinary core idea model described above and QWERTY-style arbitrary conventions that are understood by scientists but likely to be confusing to student. In particular, each model departs from the NRC recommendations in the following ways:

- Each model names particular forms of energy that are apparent in atomic-molecular, macroscopic, and large-scale manifestations.
- Each model locates energy in particular parts of a system, rather than specifically in motions of particles and fields or in states of systems as a whole.
- Each model defines "zero energy," making it possible to assign absolute values to energy present in particular parts of a system.
- Each model uses simplifying assumptions and conventions.

Table 2, below, compares four of these models, focusing in particular on how they deal with chemical energy. (The descriptions are incomplete, leaving out parts that are peripheral to the argument.)

Table 2: Comparing four conventional models of energy

Model	***Forms of energy***	***Locations of energy***	***Zero energy***	***Simplifying conventions***
1. Heat transfer	Thermal energy	Hot and cold materials	0 K (absolute 0)	Usually not used for chemical changes
2a. Hess's Law: Bond energies	Chemical energy	Chemical bonds	Independent atoms	1. Uses positive numbers to describe negative potential energies 2. Ignores other bonds, hydration, entropy, etc.
2b. Hess's Law: Molecular energies	Chemical energy	Molecules or substances	Pure elements in standard conditions	Conventional definition of zero energy for each element
3. Biogeochemical energy	Chemical energy	Pools/reservoirs of organic matter	Equilibrium with atmosphere	Associates chemical energy with being out of

				equilibrium with atmosphere

Here are some elaborations on Table 2, with the aim of noticing ways in which contradictions within and among them detract from their simplicity, parsimony, and consistency, both individually and as a group.

1. Heat transfer

In order to get energy from heat transfer, (e.g., by running a heat engine) we can't have every part of a system the same temperature. We need either a heat source—some materials that are hotter than the rest of the system—or a heat sink—some materials that are colder than the rest of the system.

Note that we could call both heat sources and heat sinks "energy sources" in that they both make heat transfer possible, but in thermodynamics we don't do that. Instead we say that heat sources have high thermal energy, that heat sinks have low thermal energy, and that the direction of energy transfer is from the heat source to the heat sink. Thus the definition of zero *available* energy (everything at the same temperature) is different from the definition of zero *absolute* energy (materials at 0K).

This distinction between available energy and absolute energy is important because we can only detect and measure available energy—the energy transfer or transformation that accompanies some change in a system. So whenever a model assigns values for absolute energy—saying how much energy a particular part of a system does or does not have—it requires a set of conventions to define zero energy and the relationships between the measurements of available energy which we can make and the values of absolute energy which we assign. As we shall see, those conventions differ in potentially confusing ways among models.

2. Hess's Law energy

In explaining energy transformations during chemical changes, we commonly rely on Hess's Law. Hess's Law is simply stated (e.g., "fact that the enthalpy of a chemical process is independent of the path taken from the initial to the final state"), but it is commonly used as the basis for assertions that are more complex and problematic. In particular, Hess's Law is commonly used to take observations we CAN make (enthalpies of chemical reactions, or available energy) as a basis for values that we CANNOT observe (chemical energy stored in bonds or molecules, or absolute energy).

Assigning energy values to bonds or molecules, rather then the observable enthalpies of chemical reactions, requires additional assumptions or conventions. In particular, it is necessary to decide what kinds of bonds or molecules will be designated as have "zero" energy. I would like to discuss two different ways of using Hess's Law that use different conventions, one of which focuses on bond energies; the other on molecular energies.

Hess's Law and bond energies. Table 2, below, was sent by one of the biology teachers to "prove" that we were mistaken in claiming that C-C and C-H bonds have higher potential energies than H-O and C=O bonds. In my experience, this teacher was typical of both the biology and chemistry majors in my methods class and the practicing teachers that I work with. Most of these teachers remember three things from their study of Hess's Law:

1. All bonds have energy (meaning positive potential energy)
2. Strong bonds have more energy
3. Breaking bonds releases energy

These beliefs seem so sensible that they have great power, and they are reinforced by lists or tables of chemical bond energies like Table 3 below. My view is that it makes about as much sense to assign positive energies to these bonds as it does to say that positive charges are moving in an electric circuit. The signs in this table, in other words, are conventions born of historical accident. It would make more sense to say that the values actually are all NEGATIVE--the difference between the energy of bonded and individual atoms. So to use these bond energies to decide whether a reaction releases or absorbs energy, you have to compare the (negative) bond energies of the reactants with the (negative) bond energies of the products

Table 3: Bond Dissociation Energies

Average bond energies, kcal/mole	
C-H	98
O-H	110
C-C	80
C-O	78
H-H	103
C-N	65
O=O	116 (2 x 58)
C=O	187* (2 x 93.5)

C=C	145 (2 x 72.5)
(* as found in CO_2)	

*Thus the C=O double bond in carbon dioxide (O=C=O) has a bond energy of 187 kcal, whereas when this bond is found as part of a larger molecule, the value is closer to 170 kcal.

Read correctly, this table shows that replacing C-H and O-H (and O=O) bonds with C-O and H-O (and C=O) bonds releases energy. Let's take burning of methane as an example. Using the bond energies from the table below:

CH_4 (4*-98 kcal) + $2O_2$ (2*-116 kcal) --> CO_2 (2*-187 kcal) + $2H_2O$ (4*-110 kcal)

So that gives us bond energies of -624 kcal for the reactants and -814 kcal for the products: 190 kcal that is released as heat and light. You will get similar results if you compare the reactant and product bond energies for the oxidation of any other organic molecule.

So a correct reading of Table 3 shows that in the burning methane example it requires energy to break the high-energy bonds in the reactants (this is the activation energy, and what catalysts like enzymes do is lower the activation energy). The energy is released from the FORMATION of the low-energy bonds in the products. This is why we are always careful in *Carbon TIME* to say that energy is released when materials go from high-energy to low-energy bonds, NOT when the high-energy bonds are broken.

Another aspect of Table 3 is more ambiguous and problematic. If you look at the bond energies in the equation above, you could argue that really most of the energy is released due to the reduction of oxygen rather than the oxidation of C and H, so that at the very least O=O should be included in the list of high-energy bonds. I would like to argue that this is mostly a matter of arbitrary convention rather than an essential characteristic of the bonds themselves.

In particular, note that the decision to assign an energy of zero to all independent atoms is purely conventional. If we think about *available* energy, it doesn't really seem to make much sense to assign all independent atoms an energy of zero. For example, some independent atoms (e.g., fluorine) can release energy by reacting strongly with many other atoms, whereas other independent atoms (e.g., neon) have no available chemical energy at all. But for practical purposes this really doesn't matter. As long as we stay consistent with this convention, we will get (approximately) correct predictions of the observations we can make—enthalpies of chemical reactions.

Table 3 supports something like the following description of energy transformations in the combustion of methane in oxygen: The reactants—CH_4 and O_2—are both described as having relatively weak (higher energy) bonds, while the products—CO_2 and H_2O—are described as having stronger, lower-energy bonds. But if we consider available energy or focus on valence electrons, there are important similarities between the chemical reaction and the heat transfer system. Methane is like a heat source—it is electropositive, meaning that it has relatively high-energy valence electrons. Oxygen is like a heat sink—it is electronegative, meaning that it has available orbitals for higher-energy electrons.

So a treatment of the combustion of methane that parallels the thermodynamic treatment of heat transfer COULD locate the energy released as initially available from the high-energy valence electrons of the methane, and that energy is released when they move to lower-energy orbitals made available from the oxygen. That's not what we normally do, of course, but I'm arguing that what we normally do is in part a matter of convention.

Hess's Law and molecular enthalpies of formation. Another way of using Hess's Law focuses on intact molecules rather than individual bonds and assigns zero energy to pure elements in standard conditions rather than to individual atoms. Figure 1, below, shows the burning of methane using these conventions (from *courses.washington.edu/bhrchem/c152/Lec05.pdf).* The author, Bruce Robinson, defines enthalpies of formation of chemical compounds as follows:

> Standard Enthalpy of Formation is "The change in enthalpy that accompanies the formation of 1 mole of a compound from its elements with all substances at standard state."

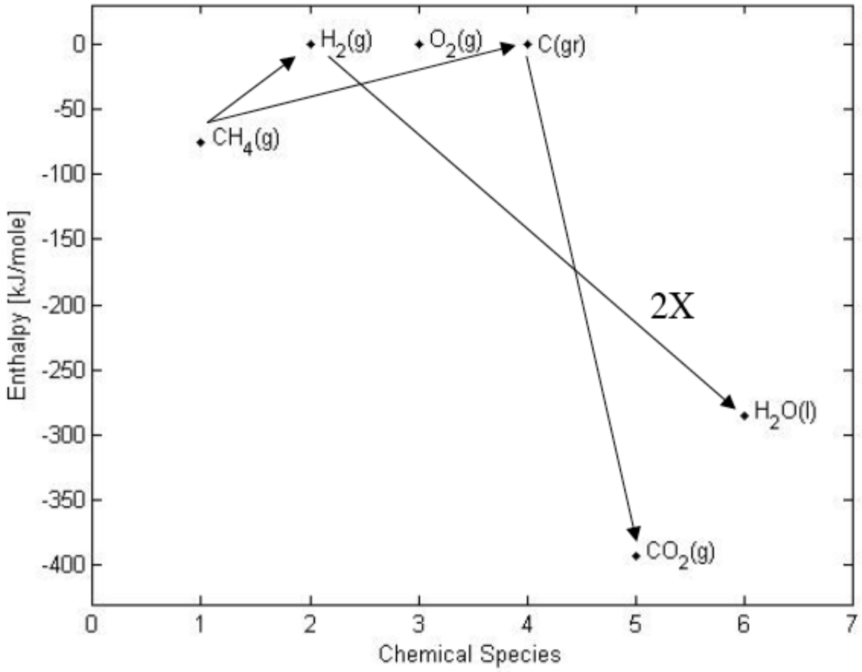

Figure 1: Energies of burning methane going through standard states

So Table 3 and Figure 1 lead to approximately the same values for the enthalpies of chemical reactions by following different procedures. Note, though, that the different conventions for defining zero energy lead to apparently different relationships among the energies of bonds. In Table 3, for example, the bonds in pure substances (C-C, H-H, O=O) all have different negative energies. In Figure 1, the energies of the pure elements are all defined as the same, and equal to zero. Once again, we see that the values we assign for absolute chemical energy (as opposed to the chemical energy available from particular reactions) depend in part of arbitrary conventions.

3. Energy flow in large-scale systems

Biogeochemists tracking chemical energy through large-scale systems *could* follow either of the Hess's Law conventions described above, saying that both O_2 and pools of organic materials (biomass, soil carbon, fossil fuels) are high in chemical energy. This would not be inconsistent with our understanding of the origins of our atmospheric oxygen—that it is a legacy of photosynthesis from previous ages, generated using energy from sunlight.

BUT that is not what biogeochemists normally do. Instead they locate chemical energy in pools of organic matter. This could be taken as an indication that they don't understand Hess's Law, but I would take it more as an indication that they have chosen different conventions for defining and measuring chemical energy.

One way of thinking about this is to say that the biogeochemists are focusing on the chemical equivalent of *available* chemical energy rather than *absolute* chemical energy. In this case, the chemical equivalent of "ambient temperature" is the Earth's atmosphere. Chemical energy is available when materials are out of equilibrium with the atmosphere. Chemical energy can be stored either because the out-of-equilibrium materials are maintained in that state by a continuing influx of solar energy or because they are sequestered—protected from contact with the atmosphere.

Here's another intriguing way to think of what biogeochemists are doing: They are implicitly using Hess's Law to define enthalpies of formation, BUT instead of formation from the elements, they are considering formation from the substances in equilibrium with the atmosphere: N_2, O_2, CO_2, and H_2O. While this is not conventional, I can think of no scientific reason why we couldn't do this. We can define the substances in the atmosphere as having zero chemical energy, then the "enthalpies of formation from oxides" would basically be heats of combustion, which tell us directly about how much energy is in an organic molecule relative to CO_2 and H_2O. Some interesting things to note here:

- The enthalpies of formation of organic molecules will now be positive (or negative—in any case, the opposite of enthalpies of formation from the elements or independent atoms).

- One way to make a rough estimate of how positive the enthalpies of formation will be is to count the number of reduced C and H (C-C and C-H) bonds in the molecules of a substance.
- This convention once again moves the chemical energy of O_2 with respect to organic materials. Now, instead of having more chemical energy than most organic materials, O_2 has less.

Back to Carbon TIME

Let me try to summarize the argument so far:

1. If we want to develop a model of chemical energy that is useful for *Carbon TIME*, we need to consider:
    a. General criteria for useful models in the science curriculum: comprehensibility, efficiency, consistency, and productivity for future learning.
    b. Specific characteristics of an energy model identified in the crosscutting concepts section of the NRC *Framework:* energy is different from matter, without mass, and conserved in physical and chemical processes
2. Evidence from learning progression research indicates that model suggested in the physical science section of the NRC *Framework*, requiring an understanding of subatomic particles and fields, does not meet the criteria of comprehensibility and efficiency.
3. Other commonly used models of chemical energy, particularly conventional applications of Hess's Law, rely on arbitrary conventions for defining energy in bonds and molecules that make them incomprehensible to our students, inefficient, and inconsistent across processes and scales.

The core question is what to do about O_2: Do we treat it as a material with high-energy bonds, consistent with conventional applications of Hess's Law, or do we use a model more like the ones used by biogeochemists to model energy flow in large-scale systems? The biogeochemical models focus more on available energy than on absolute chemical energy, identifying organic materials that are out of equilibrium we the atmosphere as our most important pools of available chemical energy.

So all things considered, I think that a version of the biogeochemical model provides the best basis for a model of chemical energy that meets all of the criteria in point 1 above. Here are some possible key elements in a treatment:

1. Identify organic substances that are out of equilibrium with the atmosphere and therefore can make energy available by reaction with O_2. Reduced carbon and hydrogen (C-C and C-H bonds) are the key evidence for those substances

2. Model the key characteristics of energy (point 1b above) by marking the evidence of available energy (C-C and C-H bonds) with twist ties and following them through carbon-transforming processes. We can say, for example, that the twist ties represent the energy available when the organic molecules combine with oxygen.
3. Make sure to explain that energy is released when low-energy bonds (C=O and H-O) are created, whereas it requires energy to break all bonds.
4. Create a student handout that teachers would have the option of using. This handout would explain that we are particularly interested in identifying chemical energy that can be made available through reactions of substances with oxygen, and we need to trace what happens to that energy.

This is unconventional, but I think it is the model that best meets all the criteria listed in 1a and 1b above.

Brainstorming: Text to explain chemical energy

Here's a draft for an optional handout that teachers could use, depending on their judgment of how they want to handle the tradeoff between simplicity and consistency with scientific convention.

Lesson 5.2: More about Chemical Energy Handout

What is chemical energy? Every atom has a small nucleus, made of protons and neutrons, and *electrons* that circulate outside the nucleus. Electrons are like other particles in that they move naturally toward low-energy places or states close to the nucleus, like balls that roll downhill.

Molecules and chemical energy exist because many atoms have either too many or too few electrons. Carbon and hydrogen have extra electrons; they could be more stable if they could get rid of or share some of their extra electrons. Oxygen, on the other hand, does not have enough electrons; oxygen atoms would be more stable if they could add some electrons.

Chemical bonds and molecules. Molecules exist because electrons can move to other atoms. When carbon and hydrogen share electrons, the shared extra electrons can move to lower-energy states. Oxygen atoms can also become more stable by gaining electrons to "fill their gaps." Atoms that share electrons stay close together, so those shared electrons are the *chemical bonds* that keep atoms together in molecules.

High-energy and low-energy bonds. Carbon and hydrogen atoms can lose a little energy (like a ball rolling a little way downhill) if they share electrons with other carbon and hydrogen atoms. But they still have their basic problem—extra electrons—so we say that C-C and C-H bonds are relatively weak *high-energy bonds*.

BUT if carbon and hydrogen atoms can give their extra electrons to oxygen atoms (remember oxygen atoms have too few electrons), then they can lose a lot more energy (like a ball rolling farther downhill). So we say that C-O and H-O bonds are stronger *low energy bonds.*

Keeping track of chemical energy. There are several methods of keeping track of how much energy is transformed during a chemical reaction. Chemists can make accurate calculations of the amount of energy by using Hess's Law. In this unit we won't try to be that accurate, though. Instead, we will be sure to notice whenever carbon atoms have *high-energy bonds that could be replaced by low-energy bonds.*

So we will use twist ties to identify high-energy C-C and C-H bonds. Those bonds have extra electrons that could lower their energy by getting close to oxygen atoms. If that actually happens—if the electrons move from C-C or C-H bonds to C-O or H-O bonds—then we can use the twist ties to remind us that energy was released in the process, and changed into some other form of energy such as heat, light, or motion.

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