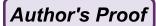
Metadata of the chapter that will be visualized online

Chapter Title	Energy in Chemical Systems: An Integrated Approach		
Copyright Year	2014		
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Corresponding Author	Family Name	Cooper	
	Particle		
	Given Name	Melanie M.	
	Suffix		
	Division	Department of Chemistry	
	Organization	Michigan State University	
	Address	East Lansing, MI, USA	
Author	Family Name	Klymkowsky	
	Particle		
	Given Name	Michael W.	
	Suffix		
	Division	Department of Molecular, Cellular and Developmental Biology	
	Organization	University of Colorado	
	Address	Boulder, CO, USA	
Author	Family Name	Becker	
	Particle		
	Given Name	Nicole M.	
	Suffix		
	Division	Department of Chemistry	
	Organization	Michigan State University	
	Address	East Lansing, MI, USA	
Abstract	"Energy" is a complex scientific concept central to all scientific disciplines. Here we describe three perspectives often used to address energy in the context of introductory college level courses: the <i>macroscopic</i> , which involves thermodynamic and mathematical treatments of energy and energy changes, the <i>atomic-molecular</i> , which relates to energy changes that result from bonding and intermolecular interactions, and the <i>quantum-mechanical</i> , which relates to energy quantization and provides the basis for understanding periodic trends, molecular structure, and electromagnetic radiation. A robust understanding of the role of energy within chemical systems requires that these three perspectives be integrated, but often they are separated into distinct sections of the course and are not explicitly connected. Moreover, prior instruction that does not explicitly address energy concepts at the molecular level almost certainly adds to student challenges. We suggest an alternate approach, illustrated by the new general chemistry course		

Author's Proof

"Chemistry, Life, the Universe and Everything", in which structure, properties and energy are presented as three interconnected learning progressions, and the treatment of energy is integrated. All three energy perspectives are explicitly addressed and related to each other in increasingly more sophisticated ways, so that students are led from the structure of the atom through to networked biological reactions, and the role that energy, entropy and Gibbs energy play in these systems.



Chapter 17 **Energy in Chemical Systems: An Integrated Approach**

Melanie M. Cooper, Michael W. Klymkowsky, and Nicole M. Becker

17.1 Introduction AO1

Students are often told that chemistry is "the study of matter and the changes 6 that it undergoes" (Chang and Goldsby 2012). What is less often emphasized is 7 that understanding chemistry depends upon an understanding of the central role 8 of energy in chemical systems. From the structure of individual atoms, to the 9 folding of complex bio-molecules; from the simplest reactions, to the cascades 10 of coupled reactions that have enabled living systems to remain organized and 11 fight the tendency to disorder, understanding energy and energy changes are key. 12 Unfortunately the central role of energy in the chemistry curriculum is often not 13 made explicit, particularly in introductory college-level courses such as general and 14 organic chemistry.

Based on a review of the literature related to students' understanding of energy 16 ideas in chemistry contexts and on our experiences with introductory chemistry 17 courses, we suggest that in introductory level college chemistry courses the concept 18 of energy is often introduced from three different perspectives: the macroscopic; 19 the atomic-molecular; and the quantum-mechanical perspectives. We discuss these 20 three perspectives and the ways they may (or may not) be connected within the 21 curriculum in the following Sections. 22

AO₂

Department of Chemistry, Michigan State University, East Lansing, MI, USA

M.W. Klymkowsky

Department of Molecular, Cellular and Developmental Biology, University of Colorado, Boulder, CO, USA

R.F. Chen et al. (eds.), Teaching and Learning of Energy in K-12 Education, DOI 10.1007/978-3-319-05017-1_17, © Springer International Publishing Switzerland 2014

17.1.1 The Macroscopic Perspective

Although temperature change is a physical manifestation of the energy changes that 24 take place on the atomic-molecular level, most instructional approaches to college- 25 level chemistry do little to emphasize these origins: they do not explicitly connect 26 the macroscopic (temperature) to the microscopic and molecular. For example, 27 students might discuss energy changes of endothermic or exothermic reactions 28 that are reflected by observable changes in temperature before ideas of molecular 29 structure are introduced. Such energy changes are typically organized under the 30 general headings of "Thermochemistry" or "Thermodynamics". Thermochemistry 31 is concerned with the energy changes that take place when a macroscopic chemical 32 system undergoes change, and usually these changes are observable as changes 33 in temperature. For most students, learning thermodynamics topics in a general 34 chemistry course begins with calculations using specific heats and temperatures, 35 which are then related to enthalpy (H). Later (usually in the second semester general 36 chemistry course), other thermodynamic functions such as entropy (S) and Gibbs 37 energy (G) are also introduced, and while more abstract than observable changes 38 in temperature changes, these functions also are related to changes in energy of 39 macroscopic systems.

Change in Gibbs energy, for example, is a thermodynamic state function that 41 is often represented by the equation $\Delta G = \Delta H - T\Delta S$ (where ΔH is the enthalpy 42 change of a reaction, T is the temperature, and ΔS is the entropy of the system). 43 This function is important in that is serves a proxy for the Second Law of 44 Thermodynamics, allowing one to make predictions about the spontaneity of a 45 process using only variables related to the system in question. Unlike enthalpy and 46 internal energy, Gibbs energy is not conserved (because it includes an entropic 47 term). Gibbs energy is one of the most important and useful thermodynamic 48 functions because it allows predictions to be made about the direction of change. 49 Biologists, for instance, might use the Gibbs function to determine the direction of 50 change in biological systems and to understand how coupled reactions can drive 51 thermodynamically unfavorable processes.

However, there is evidence that traditional approaches to teaching thermodynamics topics may leave students with fragmented or even incorrect understandings 54 about what thermodynamic variables represent and how they relate to macroscopic 55 changes in energy that correspond to changes in chemical systems. For instance, 56 prior literature related to students' understanding of Gibbs energy suggests that 57 students may not develop an understanding of Gibbs energy as a proxy for the 58 Second Law of Thermodynamics. Instead, students may conflate change in Gibbs 59 energy for a process, ΔG , with the amount of heat transferred in or out of a 60 system (Thomas and Schwenz 1998) or they may believe that the magnitude of 61 ΔG can be used to determine the rate of reaction (Sozbilir 2002). Factors such 62 as entropy (S), which is often discussed in conjunction with energy changes in 63 macroscopic systems, can be further sources of confusion. While entropy is best 64 understood as related to the number of states or arrangements possible within a 65



system (Lambert 2002), students may conflate entropy and energy (Carson and 66 Watson 2002), believing that entropy represents a form of energy.

We believe that such difficulties may be related to the fact thermodynamic treatments of energy in introductory chemistry coursework seldom build on students' 69
prior knowledge, but rather introduce a new set of ideas that are not linked to other 70
knowledge and may appear to the student to be introduced solely for the purpose 71
of doing calculations rather than as a foundation upon which to predict molecular 72
behaviors. 73



Representational Difficulties Related to Macroscopic Perspectives on Energy

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In addition to the fragmented nature of energy topics within chemistry curricula, the 76 representational tools used to communicate energy ideas may contribute to student 77 difficulties with energy topics. As Taber (2013) noted, "Learning chemistry involves 78 both forming concepts that are sufficiently aligned with those of other members 79 of the chemical community, *and* adopting the systems of symbols commonly used 80 within the chemical community so as to be able to communicate with others about 81 these concepts" (p. 4). Thus, students must develop fluency with representational 82 resources commonly encountered in introductory chemistry classes, such as mathematical expressions and graphical representations. Mathematical representations 84 are especially important the use of mathematical resources to model and represent 85 systems is a key scientific practice that has the potential to facilitate students' 86 understanding of energy transfer and conservation in more complex systems 87 (National Research Council 2012).

However, there is abundant evidence that students approach mathematical representations of thermodynamic functions, such as enthalpy or Gibbs Energy, in an algorithmic fashion and that even advanced chemistry students can fail to grasp what these mathematical representations of functions represent. For instance, a practicing schemist might be able to examine an equation such as U=q+w and interpret it a representation of idea that the total energy of a system is the combination of heat and work done on the system, and as a representation of the conservation of energy. Students, however, may struggle to relate variables such as heat and work to the real-world phenomena or atomic-molecular level understandings of the system. For example, Hadfield and Wieman (2010) found that students enrolled in an upperdivision physical chemistry course did not consider the expression U=q+w to serious relate to the conservation of energy.

These difficulties may derive in part from the fact that students' everyday 101 interpretations of energy-related terminology (for example "heat" or "work," both 102 of which are commonly used in everyday speech) may be quite inconsistent with 103 the way those terms are appropriately used in thermodynamic contexts (Jin and 104 Anderson 2012; Kaper and Goedhart 2002; Lancor 2012). Thus to successfully 105 interpret expressions such as U = q + w students must not only be able to interpret 106 the mathematical expression, but hold understandings of terms like "energy", 107

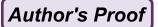
"heat", and "work" that are consistent with disciplinary understandings of those terms (Jewett 2008). This is particularly problematic since if students do not develop an appreciation of the concepts underlying thermodynamic functions, we feel it becomes nearly impossible for students to appreciate energy as a tool that they may use to predict and explain the outcomes of chemical processes.

17.1.2 The Atomic-Molecular Perspective

Energy concepts are critical to understanding how molecules form and behave and it is at the atomic-molecular level where the origins of the observable manifestations of energy change can be observed. As such, a second perspective on energy in the introductory chemistry curriculum often relates to energy at the atomic-molecular level in the context of the structure and interactions of matter.

Energy associated with bonding and intermolecular interactions are foundational 119 parts of chemistry in that they enable predictions of molecular properties and 120 energy transformations at the macroscopic level. It is possible to explain most 121 of the properties and interactions of matter, ranging from the sizes of atoms to 122 their interactions along the spectrum from London Dispersion Forces to covalent 123 bonding, in terms of kinetic and potential energy. To understand bonding at a 124 conceptual level in terms of energy, students must recognize that such interactions 125 are based on attractive and repulsive forces, and that a stable interaction is formed 126 when there is a balance between these forces, an "energy minimum" (Nahum 127 et al. 2007). However, developing the ability to reason about energy at the atomicmolecular scale is not without difficulties. In reasoning about bond formation and 129 stability, students may rely on heuristics such as the octet rule, rather than an understanding of how electrostatic forces contribute to bond formation (Taber 1998). 131 Students may view ionic bonds, covalent bonds, and intermolecular interactions as 132 distinct entities rather than understanding that all involve electrostatic interactions 133 and energy minimization (Taber 1998). Furthermore, misconceptions related to the 134 energetics of bonding interactions, such as the idea that bonds "store" energy and 135 that energy is released when a covalent bond is broken are persistent sources of 136 confusion. A number of researchers have found that even after instruction, typically 137 over 50 % of students incorrectly believe that bonds release energy when they are 138 broken (Barker and Millar 2000; Boo 1998).

While the construct of potential energy is often referenced when discussing 140 intermolecular forces and bonding, chemistry curricula rarely address how electrostatic potential energy at the molecular level, which arises from electrostatic 142 interactions, relates to the more familiar concepts such as gravitational potential energy. Unfortunately at present most students arrive at college having been exposed 144 to kinetic and potential energy in macroscopic systems (for example a ball rolling 145 down a hill), but in our experience, they have little understanding of how these ideas 146 might translate to the molecular level. It is our hope that as students who experience 147 instruction that builds upon the NRC Framework for Science Education (NRC 2012) 148



and the Next Generation Science Standards (NGSS) (Achieve 2013), they will 149 develop a more coherent framework upon which to build some of these ideas. The 150 NGSS emphasize the idea that energy is best treated in an interdisciplinary manner. 151 with explicit connections between the macroscopic and the atomic molecular level. 152 For instance, one connection that may be made is that electrostatic potential energy 153 can be considered analogous to gravitational potential energy in that both depend 154 on the distance between two interacting objects, both involve forces that mediate 155 interactions between objects, and the equations relating the energy of both interactions take very similar forms. If students understand these similarities, they may 157 be better equipped to differentiate gravitational potential energy from electrostatic 158 potential energy in atomic-molecular systems. For example, electrostatic potential 159 energy in the context of molecular systems differs from gravitational in that it is a 160 far stronger interaction at the molecular level and there are two types of charges, 161 meaning that there can be both attractive and repulsive forces, while only attractive 162 forces are present within a gravitational field. Introductory chemistry texts often do 163 not explicitly acknowledge the similarities, differences and difficulties in translating 164 across scales from the macroscopic to the molecular and students are largely left to 165 infer these for themselves.

We consider the origin of potential and kinetic energy changes at the atomicmolecular level critical to understanding the basis of thermodynamic ideas that are
in common use. If students do not know how energy is transferred and stored at the
atomic-molecular level, they will likely find it difficult to understand, for example,
the origin of "chemical energy" – how or why chemical reactions can be used
the origin of "chemical energy" – how or why chemical reactions can be used
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17.1.3 The Quantum-Mechanical Perspective

The third focus of energy instruction in university-level general chemistry courses centers on the idea that energy is quantized at the atomic-molecular scale. For most students (and for most people!) this idea is entirely counterintuitive as it has no counterpart in the macroscopic, observable world. Energy quantization is often taught in introductory chemistry courses primarily in connection with topics related to atomic structure. However, connections between quantization of energy from a quantum-mechanical perspective and atomic-molecular or macroscopic henomena are seldom explicit. Rather than asking students to use the idea of energy quantization to explain phenomena such as why carbon, the building block of life, forms four bonds and not six, or why materials emit or absorb electromagnetic radiation of particular wavelengths, we typically emphasize more easily assessable ideas such as the recitation of electron configurations.

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Again, there are a number of reports in the literature about students' under- 190 standings of the concepts of quantum chemistry (Taber 2002, 2004; Tsaparlis and 191 Papaphotis 2009). Despite instruction, students may fail to grasp the relationship 192 between energy quantization and orbital ideas in general chemistry contexts (Park 193 and Light 2009; Taber 2002). Park and Light (2009) described the quantization 194 of energy and the uncertainty principle as "threshold concepts". Clearly, if we 195 want students to be able to cross this "threshold" and to relate energy ideas from 196 the quantum-mechanical perspective to molecular-level structure as well as to 197 macroscopic phenomena, more explicit attention is needed towards helping students 198 connect energy ideas across the chemistry curriculum.

In summary, introductory college chemistry courses typically "cover" energy 200 ideas from three perspectives: macroscopic, atomic-molecular, and quantum 201 mechanical. However, in the context of most traditional courses, we feel such 202 coverage may be fragmentary, not connected to students' earlier knowledge, and 203 typically not set in a meaningful context.

How Should General Chemistry Students Learn About 17.2 **Energy Within an Introductory Chemistry Context?**

It is clear from our analysis of traditional approaches to teaching energy con- 207 cepts within the chemistry curriculum that the three dominant perspectives on 208 energy, macroscopic, atomic-molecular, and quantum-mechanical, are rarely well- 209 integrated. Indeed, there is ample evidence that students lack a coherent framework 210 of energy concepts on which they can hang their understanding of energy changes 211 associated with chemical change. While multiple perspectives on energy clearly 212 have their place within the curricula, more must be done to help students connect 213 energy ideas across the curriculum.

The problems inherent in traditional approaches to energy instruction are exac-215 erbated by the fact that most assessments in traditional chemistry courses still 216 emphasize rote problem solving and factual recall over conceptual understanding, 217 and there may be little opportunity for students to synthesize and connect energy 218 ideas across the curriculum. Many of the leading textbooks for general chemistry 219 introduce energy topics in different orders (there are even editions of the same text 220 with the topics juggled), so it is clear that there is no consensus on how to develop 221 and connect energy concepts or even why they are important.

We believe that energy ideas must be developed in a scaffolded progression, 223 which helps students to make sense of energy phenomena across macroscopic, 224 atomic-molecular, and quantum mechanical levels. Our approach to designing an 225 energy learning progression for general chemistry aims to reconcile these different 226 perspectives and explicitly recognize places where energy is best treated by one 227 or more of the perspectives. Our goal is to help students develop an integrated 228 understanding of energy concepts that can help them make connections between 229 the three perspectives discussed here.

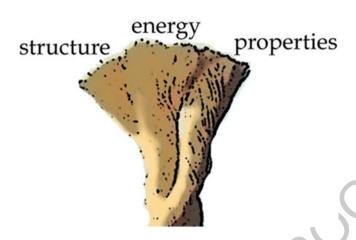


Fig. 17.1 The interconnected learning progressions of structure, properties and energy



chemical systems.

The CLUE Approach to Energy in Chemical Systems

Our current work in this direction centers on developing, teaching and assessing the 232 outcomes for a new general chemistry curriculum: Chemistry, Life, the Universe 233 and Everything (NSF DUE # 0816692). This approach is organized around 234 three interconnected learning progressions for core ideas; Structure, Properties and 235 Energy, which are represented in Fig. 17.1 by three intertwined, interconnected 236 strands. As each core idea is developed, its connections to the other core ideas 237 are also emphasized. Our intent is to develop and connect structure, properties and 238 energy throughout the course, rather than treating them separately. Figure 17.1 is 239 intended to show how these strands are both intertwined and interconnected. The 240 curriculum is structured so as to progress from simple systems, such as the atomic- 241 level interactions of atoms and molecules, to more complex systems such as the 242 networked reactions that drive thermodynamically unfavorable processes. At each 243 stage in the curriculum, the three perspectives on energy are coordinated (Fig. 17.2) 244

in order to give students access to a comprehensive view of the role of energy in 245

We have previously reported on assessments of learning outcomes for the 247 structure-properties learning progression within the CLUE curriculum (Cooper et al. 248 2012). Here, we provide a description of the design of the progression and the 249 connections among ideas that support the development of a more integrated and 250 robust conceptual framework for energy as it is needed to understand chemical 251 systems. Research on student learning outcomes for the energy learning progression 252 is underway and will be reported elsewhere.

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¹Selected course materials for the course available online at http://besocratic.colorado.edu/CLUE-Chemistry/index.html

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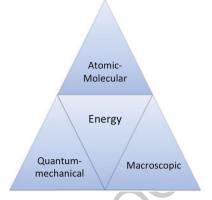
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Fig. 17.2 Three perspectives on energy in the CLUE chemistry cours



While the initial development of the curricular materials pre-dated the release of 254 the NRC Framework for STEM education (NRC 2012), the approach we describe 255 here closely parallels many of the disciplinary core ideas related to energy in the 256 physical sciences in the Framework. For example the Framework recommends a 257 more coherent approach to the teaching of energy:

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 Framework also states that:

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).

While to date there is little empirical evidence that suggests that learning about 267 molecular-level energy changes prior to learning about macroscopic energy changes 268 in chemical systems is beneficial for students, we believe that this approach has the 269 potential to addresses major impediments to student learning and to meet students 270 where they are in terms of prior knowledge. Students who enroll in college to study 271 STEM fields have already learned about the existence of atoms in K-12 coursework 272 and it is highly likely that they have also been exposed to ideas about energy and 273 energy changes at the macroscopic level. Ideally, students would come to college 274 with a firm grasp of macroscopic energy ideas, including the relationships between 275 different "kinds" of potential energy (gravitational, electrostatic, magnetic). Unfor- 276 tunately at the moment this does not appear to be the case, and we must address 277 energy in ways that are appropriate for understanding of foundational chemistry 278 principles. While students' prior knowledge related to energy ideas at the atomic- 279 molecular level may often be fragmented and incomplete, we believe that beginning 280 with a discussion of energy at the atomic-molecular level with explicit connections 281 to their prior understanding of energy ideas at the macroscopic level has the potential 282 to serve as a foundation for better understanding discussions of macroscopic energy 283 changes.



Thus, our current work centers the development of a learning progression that 285 begins with discussion of energy ideas at the atomic level and connects to quantum- 286 mechanical and macroscopic descriptions of energy. In the following sections, we 287 present an overview of this progression and illustrate the ways in which energy ideas 288 are integral within the course structure by using examples from the two-semester 289 general chemistry sequence.



17.2.1.1 Chapter 1: Atoms

The CLUE approach to energy begins with an introduction to atomic structure 292 and interactions in their simplest form. That is, quantization of energy levels is 293 not the starting point of this introduction; rather we aim to link to students' prior 294 knowledge about energy and interactions at the macroscopic-level by appealing 295 to students' understanding of gravitational force and energy minimization at the 296 macroscopic level. We begin by asking students what they know about energy 297 both in the macroscopic "real world" and at the molecular level, and through 298 class discussions begin to connect the two perspectives. We emphasize both the 299 similarities between the gravitational forces and energy changes they have learned 300 previously (for example a roller coaster ride), and the electromagnetic force that 301 causes attractions and repulsions at the atomic-molecular level.

Throughout the CLUE curriculum, we use a number of activities in order to help 303 students engage with the material. For instance the web-based simulation² shown 304 in Fig. 17.3 uses the interactions of helium atoms as a simple model for reasoning 305 about the potential energy changes that result from atomic-molecular interactions. 306 The screenshots in Fig. 17.3 show a plot of potential energy versus distance between 307 the nuclei and two bars representing the kinetic and the total energy of the system. 308 As students interact with the simulation, for example by changing the distance 309 between the helium atoms, they are prompted by the simulation to consider various 310 energy changes that result from the changes they observe. The idea of energy 311 conservation is introduced by drawing students' attention to the fact that total energy 312 of the two-atom system remains constant as the atoms interact even though as the 313 fluctuating dipoles in the electron clouds attract one another, the potential energy of 314 the system decreases and the kinetic energy increases.

The activity also introduces the idea of energy minimization in chemical systems. 316 That is, a system will adopt the lowest potential energy configuration unless another 317 source of energy is added. In this case, the lowest energy configuration occurs as 318 the helium atoms interact through London Dispersion interactions. A third atom can 319 be introduced that can either accept energy and stabilize the interaction or transfer 320 energy to the two atom system.

We conclude Chapter 1 with a comparison of the energy changes associated with 322 the formation of different types of intermolecular interactions. For example, we 323

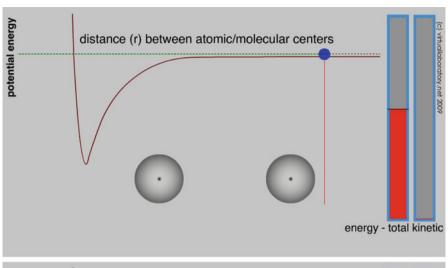
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²Available online http://besocratic.colorado.edu/CLUE-Chemistry/activities/ LondonDispersionForce/1.2-interactions-1.html

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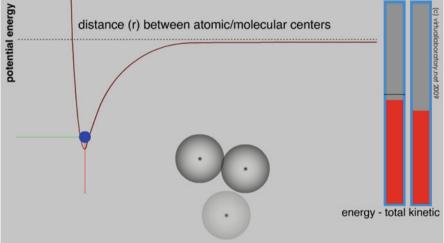
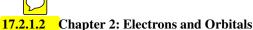


Fig. 17.3 Screenshots of the interactive simulations designed to provide students with atomicmolecular level visualizations of potential and kinetic energy and energy transfer. In the second screen shot, energy has been transferred to the "third" atom, allowing the initial pair to stabilize

compare the energies associated with interactions between helium atoms caused by 324 London Dispersion Forces (LDFs) and contrast these with the energy changes that 325 occur as a covalent bond is formed between two hydrogen atoms. Throughout the 326 CLUE curriculum, bonding and intermolecular forces are treated as a continuum of 327 interactions that minimize potential energy in the system. As suggested by others, 328 this approach may be beneficial since it exposes students to the commonalities in 329 various types of interactions between atoms and molecules (Nahum et al. 2007).





In Chapter 2, we continue our discussion of bonding and intermolecular interactions 332 by introducing the idea of quantization of energy levels at the atomic scale. 333 However, rather than emphasizing memorization of electron configurations and 334 shapes of electron orbitals, energy quantization is emphasized as an explanatory 335 principle. Using different type of assignments, e.g. in class worksheets, homework assignments and on exams, students are asked to use the idea of quantized energy 337 levels to explain phenomena such as atomic emission and absorption spectra and 338 to help explain periodic trends such as effective nuclear charge (from which other 339 periodic trends such at atomic radius, ionization energy, electronegativity and 340 reactivity can be deduced). The introduction of quantized electronic energy levels 341 also facilitates a discussion of the role of core and valence electrons, which can be 342 used to reason about ideas such as why carbon has four valence electrons available 343 for bonding (as opposed to six). These ideas provide a basis for discussion of 344 bonding models in Chapter 3.



17.2.1.3 Chapter 3: Elements, Bonding, and Physical Properties

In Chapter 3, both valence bond and molecular orbital models of bonding are 347 introduced. Again energy concepts are central to understanding the causes and 348 effects of bond formation between atoms. Bonding models are explicitly compared 349 in order to provide examples of different aspects of molecular structure for which 350 each is appropriate. The CLUE curriculum emphasizes how a model of quantized 351 molecular orbital bonding and anti-bonding orbital energies enables explanations 352 related to physical properties. Using this model, students are asked to predict and 353 explain observations such as why diamond is hard, translucent and has a very 354 high melting point, while graphite is soft, shiny and conducts electricity, while 355 also having a high melting point. Again in this chapter, the role of electrostatic 356 interactions that lower the energy of the system, and the idea that these energies 357 are quantized, are emphasized. A major aim of this chapter is to have students 358 understand the idea that bond formation releases energy from the system, and bond 359 breaking requires energy input. 360



Chapter 4: Heterogeneous Compounds

In Chapter 4, we emphasize the relationship between structure of molecules 362 and their interactions. That is, we return again to ideas that were introduced in 363 Chapter 1 about atomic interactions, and revisit them in the context of more complex 364 systems. Much of this material is concerned with helping students understand 365 the formalisms of depictions of molecular structures and to learn to decode the 366 information they contain. It is not until students have had considerable practice 367

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working with depictions of molecular-level structure that we begin examining the 368 impact of molecular-level structure on energy changes and physical properties 369 at the macroscopic level. The role of energy minimization in determining the 370 arrangement of atoms in molecules is highlighted as central to molecular-level 371 interactions. We choose to emphasize this idea and language because it is what 372 students will encounter in subsequent chemistry courses where energy minimization 373 is an important concept.



17.2.1.5 Chapter 5: Systems Thinking

Chapter 5 introduces a thermodynamic perspective on energy changes and aims 376 to connect the bulk properties of substances with molecular level interactions. We 377 begin with the concept of phase changes, since only changes in intermolecular 378 interactions are involved. At this point in the semester, students have already worked 379 with the idea that to change from a solid to liquid or a liquid to gas, energy must 380 be put into the system (and conversely that to change from gas to liquid, or liquid 381 to solid a release of energy to the surroundings must take place). They have also 382 encountered the idea that the stronger the attraction between the particles, the more 383 energy is required to overcome the interactions between them. We aim to link 384 this prior knowledge related to atomic-molecular and macroscopic energy ideas 385 by introducing further detail about associated changes at the atomic-molecular and 386 quantum mechanical perspectives. For instance, we discuss how adding thermal 387 energy may result in an increase in temperature by increasing the kinetic energy 388 of the particles, but that thermal energy may also causes increases in vibrational and 389 rotational (quantized) energy levels which do not contribute to observed temperature 390 changes.

At this point, the state function enthalpy (H) is introduced as a representation of 392 the thermal energy of a system at constant pressure. Introduction to the enthalpies of phase changes and specific heats of substances allows for a quantitative discussion 394 of ideas related to heat transfer and bond energetics. Systems at constant volume are 395 mentioned but not emphasized at this point since most students will not encounter 396 such systems in subsequent coursework. Using this approach, we are now able to 397 address the idea of atomic-molecular interactions using the three perspectives on 398 energy change as shown in Fig. 17.4.

Next, we introduce the term entropy using a probabilistic approach that is 400 grounded in a discussion of changes at the molecular level (Lambert 2002). We also 401 introduce the state function entropy (S) and the Second Law of Thermodynamics, 402 which states that the entropy of an isolated system always increases as the system 403 evolves towards the more probable state in which energy is dispersed.

Gibbs energy (G) is then introduced as a proxy for the total entropy of the 405 universe. We avoid the definition of Gibbs energy as the energy available to do work, 406 since the term "work" at the molecular level is not a very useful concept, especially 407

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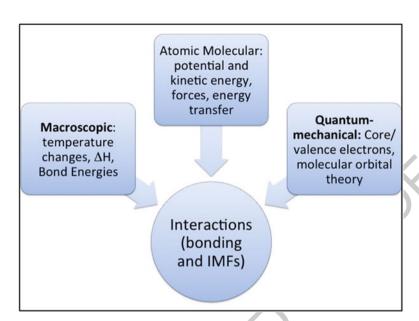


Fig. 17.4 Three perspectives on energy changes and interactions

since it is often reserved for expansion work, for example during gas evolution. 408 Instead, we emphasize the usefulness of the Gibbs energy function for predicting 409 the direction of change in a chemical system and highlight the relationship between 410 a negative Gibbs energy change and a positive total entropy change in order to 411 illustrate the role of Gibbs energy as a proxy for total entropy.

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Our objective in teaching thermodynamics topics in this way is to allow students 413 to think about energy inputs and outputs as well as the molecular and macroscopic 414 consequences of these energy changes. In concert with the concurrent development 415 of an understanding of molecular structure, this approach is designed so that 416 students may construct a coherent framework that allows them to predict and explain 417 the direction of change in a chemical system. It is intended to provide a basis 418 for understanding why some chemical processes require energy input and some 419 produce energy, and how thermodynamically unfavorable processes can be driven 420 by coupling them through common intermediates to more favorable processes. 421 Figure 17.5 illustrates the ways in which molecular, quantum mechanical, and 422 macroscopic energy ideas contribute to this framework.

The ideas developed in the first half of this curriculum are then used in the 424 second semester to understand how energy (and structure and properties) affect the 425 formation of solutions (Chapter 6), chemical reactions (Chapter 7), rate and extent 426 of chemical reactions (Chapter 8), and how networked reactions can be used to drive 427 thermodynamically unfavorable processes (Chapter 9).

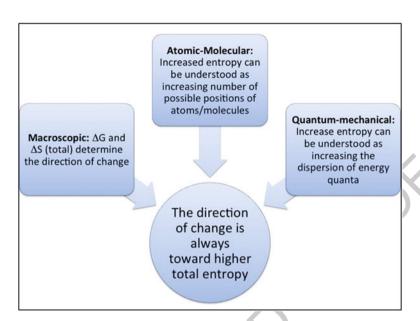


Fig. 17.5 Understanding the direction of change requires all three dimensions

17.3 Summary and Conclusions

We view energy as an integral component of introductory college level chemistry 430 courses that has the potential to provide a framework for understanding both 431 how and why chemical changes occur. As currently implemented within typical 432 introductory chemistry courses, the discussion of energy is fragmented and rarely 433 makes explicit connections across the various energy topics in the curriculum. This 434 makes it exceedingly challenging for students to build on prior knowledge since 435 most of the ideas that students have are based on macroscopic understandings of 436 energy and energy changes.

The learning progression for energy that we have described aims to explic- 438 itly connect three commonly used perspectives related on energy (macroscopic, 439 atomic-molecular, and quantum mechanical). Table 17.1 summarizes topics in the 440 curriculum where the perspectives to energy instruction may be used.

By sequencing our discussion so as to begin with a discussion of atomic structure and by connecting new topics to prior understandings, we aim to scaffold students' ability to reason about the networked reactions that drive thermodynamically unfavorable processes. The development of this learning progression and assessment of student outcomes are ongoing, with data collected from student performances and interviews being used to refine and revise this approach.

What is clear is that in chemistry we cannot continue to treat energy concepts 448 as if students already have a robust framework to build on. We must take time to 449



Table 17.1 Three perspectives on energy and phenomena that they explain

Atomic-molecular perspective needed for:	Quantum-mechanical perspective needed for:	Macroscopic perspective needed for:	
Interactions leading to potential energy minimization	Interactions of matter and electromagnetic radiation	Physical manifestations of molecular level energy changes	t1.1
Energy transfer by collisions	Energy transfer by electromagnetic radiation	Thermochemistry and thermodynamics	t1.2
Chemical and physical changes as systems	Periodic trends (effective nuclear charge etc.)	Temperature changes and chemical and physical processes	t1.3
The origins of "chemical energy"	Valence and core electrons	Gibbs energy as a proxy for the second Law of Thermodynamics, and a predictor of change	t1.4

reach back and reconstruct and re-develop energy ideas beginning at the molecular level and we must design and construct meaningful activities and assessments that encourage students to relate understandings of energy across the curriculum. 452

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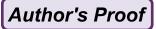
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