Using Enhanced Molecular Dynamics Models to Understand Light-Matter Interactions

Robert Tinker[1], Amy Pallant[1], Qian Xie[1] , and Ed O'Sullivan[2]

Suggested running head: **Modeling Light-Matter Interactions**

rtinker@concord.org
25 Love Lane, Concord, MA 01742
978-405-3222

---

[1] The Concord Consortium, Concord, MA.

[2] Chemistry, Parkland College, Champaign, IL

Abstract

This paper reports a study of how students arrive at an understanding of the interactions between light and matter at the atomic scale when they use a well-designed activity that features sophisticated computational models adapted for education. Previous research demonstrates the effectiveness of using computational modeling environments across many areas of science learning (Feurtzeig & Roberts, 1999), and specifically for atomic-scale phenomena (Pallant & Tinker, 2004). This work explores how computational models based on a particle model of light can support student learning of concepts such as color, photon emission, absorption spectra, fluorescence, black-body radiation, and quantum yields.

Key Words: Light and matter interactions; models; molecular dynamics; spectrum; classroom studies

Introduction: Why model light and matter interactions?

Connecting the macroscopic and atomic scales is one of the great challenges of science education. When it is possible to make these connections, students should be able to gain an explanatory framework that will reduce the amount of memorization required and help make science appear more connected and rational. In many situations, the macro-atom connection is obscured by properties that emerge at intermediate scales (mesoscales). For instance, the strength of steel, a macroscopic phenomenon, is related to the inter-atomic attraction of iron atoms, an atomic-scale phenomenon, but also depends on crystal imperfections and boundaries, nano-scale phenomena.

The color of objects and the effect of light on matter provide unusually direct connections between perceptions at the human scale and atomic-scale phenomena. Starting with only a few basic atomic-scale concepts, it is possible to explain a wide range of easily observed light phenomena that are usually ignored at the introductory level or not connected into an explanatory framework. Observable phenomena that can be explained by atomic-scale interactions include color, light absorption, emission spectra, thermal radiation, radiation heating, fluorescence, phosphorescence, and lasers.

The Science

In order to appreciate the atomic-scale mechanisms for these phenomena, it is necessary to understand some principles that determine the interaction of light with atoms and molecules. Light interactions with atoms generally require a particle view of light in which light behaves as if it consists of discrete particles called photons rather than waves. The wave-particle duality might challenge students, but it can be handled without getting sidetracked by simply treating the photon-atom interactions as fundamental properties of light. The particulate description of light and the direct manner in which photons interact with atoms provides a mechanistic framework with great explanatory power. The basic rules that determine light-matter interactions are the following:

1. Photons are massless, but have energy that is proportional to their frequency and inversely related to their wavelength.
2. The electrons bound to atoms and molecules are confined to certain discrete orbitals, each of which has a specific energy level.
3. When the energy of a photon matches the energy difference between an electron's current state and that of a higher energy state, and the photon approaches the electron, the photon is absorbed and its energy excites the electron from the lower energy state into the higher one.
4. An electron can also be excited mechanically, by capturing kinetic energy caused, for instance, by a collision with another atom or molecule.
5. An excited atom can spontaneously drop from its current energy level to a lower one and emit a new photon with energy equal to the difference between the energies of the two levels. This is the reverse of photon absorption.

6. An excited atom can drop to a lower energy level and convert the energy gained into motion of the atom. This is the reverse of mechanical excitation.

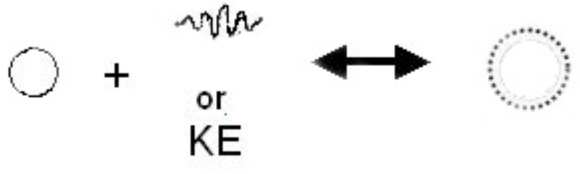

Figure1. A Symbolic Summary of Light-Atom Interactions. The circle represents an atom. An atom can gain energy (represented as a circle with dashed line around it) by absorbing a photon (represented by a squiggle) or some kinetic energy (KE). After some time, the excited atom will de-excite and generate a photon or some kinetic energy.

The transformations described in rules 3-6 must all conserve momentum and energy. These rules, when operating on groups of atoms, can explain a wide range of phenomena that students can understand as a result of experimenting with computational models.

The Role of Modeling

Learning activities based on computational models provide an alternative way to teach a wide variety of concepts. Our approach features contextual teaching and learning (Hallden, 1999; Heering & Osewold, 2007; Johnson, 2001; Parnell, 2000; Sears, 2002) that has many of the features of hands-on learning. Because the models generate visualizations that are computed in real time based on initial conditions, rules, and geometries that can be easily changed, students can choose from an infinity of different conditions, just as they can in a real lab. In our learning activities, the computed visualizations are not viewed passively like pre-recorded movies, but are, instead, highly interactive (Horwitz & Christie, 2000). Students learn by experimenting with different conditions and quickly seeing the effect of their choices in the dynamic visualizations, graphs, or other representations (Bransford, Brown, & Cocking, 2000; Krajcik, Marx, Blumenfeld, Soloway, & Fishman, 2000; Slotta, 2004). To avoid having students either skimming over the models or getting lost in all the options, our materials provide various kinds of guidance and scaffolding (Feurtzeig & Roberts, 1999; Tinker & Horwitz, 2000).

There is strong research support for interactive model-based instructional designs that focus more on teaching deeper concepts (Berenfeld & Tinker, 2001; Clement, 2000; Linn, Lee, Tinker, Husic, & Chiu, 2006). Many core science concepts can be taught effectively using interactive models of atomic and molecular systems (Clark & Jorde, 2004; Feurtzeig & Roberts, 1999). Student explorations of these models can lead to a good understanding of connections between atomic-scale events and macroscopic phenomena (Berenfeld & Tinker, 2001; Buckley, et al., 2004). Interactivity creates the rich, highly associated mental networks of concepts that we know contribute to lasting understanding (Jackson, Stratford, Krajcik, & Soloway, 1996; Snir & Smith, 1995). Our research shows that this kind of understanding can link together topics that appear quite different, reducing the cognitive load and conveying a more accurate picture of the nature and structure of science (Pallant & Tinker, 2004; Tinker, 2007a, 2007b).

Modeling Light-Matter Interactions in the *Molecular Workbench*

In order to provide a highly interactive simulation environment for student exploration of light-matter interactions that include thermal effects, we have extended the molecular dynamics modeling engine in the *Molecular Workbench (MW)* to include atom-photon interactions described in the six rules above.[3]

In *MW*, photons appear as packets of energy that are massless, uncharged, traveling in straight lines, and represented by a squiggle with a small arrow at their heads to indicate the direction of travel. The frequency associated with a photon is represented by the number of waves shown in the squiggle. Photons of higher frequency and energy are shown with more waves and photons of lower frequency and energy have fewer waves. The representation is intended to symbolize the wave-particle duality of light. Moreover, photons with energy in the visible range are shown in the appropriate color of the spectrum from red through violet; infrared and ultraviolet photons are shown in black dashed lines.

Figure 2. A beam of photons of various energies, all heading in one direction. The photons in the visible part of the spectrum are shown here with solid lines and are represented in color in

---

[3] The *Molecular Workbench* software can be found at http://workbench.concord.org/

the simulation. The photons in the invisible ranges (infrared and UV) are represented here with dashed lines and are black in the simulation.

MW provides a light source that radiates photons into the model container. The light intensity is represented by the rate of photons flowing through the model. The number and energy of excited states of a type of atom can be set graphically in an energy level diagram. An excited atom is indicated by a dashed line surrounding the atom. The user or activity author can set many of the parameters that control the interactions, such as the energy of excited states, the number of incident photons, and the temperature of the atoms. To explore the model, students run the model and the computational engine generates the subsequent states of the system based on the parameters and starting conditions. The evolving model is shown graphically together with live outputs such as graphs and gauges. A typical run requires a short period of time (less then 30 seconds) and can be rewound, stepped through, and saved in various forms.

As with any educational model, the primary goal is to foster understanding, even if some degree of accuracy must be sacrificed. It is, therefore, important to point out the simplifications used in the model. In order to show the interactions of light and matter, the scales needed to be adjusted in important ways. First, the scale of the actual wavelength for visible light is actually about 10^4 times longer than the waves shown in the model. Second, the actual speed of light is about 10^4 times faster than the speed of the photons in the model. In effect, *MW* models a world that has different values for Planck's constant and the speed of light. Electron transfer and excited states of molecules have not yet been implemented.

Classroom Studies

The Molecular Workbench team at the Concord Consortium developed a scaffolded learning activity using the extended *MW* environment called *Light and Matter Interactions*[4] designed for high school and community college students. A pilot version of the activity was tested in three community college general chemistry classes. The activity required one class lasting approximately 50 minutes. A pre-test was administered immediately prior to implementation and a post-test upon completion. In one class students had just completed an introduction to the topic during the lecture period. The other two classes studied light-matter interactions a week and a half prior to interacting with the model-based activity. Each student had his/her own computer to execute the activity.

The Light and Matter Interactions Activity

To draw students into the study of the interactions of light and matter, the activity introduces the idea that light plays an important role in many current technological innovations. The activity engages students in discovering though guided exploration basic concepts about light, the properties of photons, and the full range of the electromagnetic spectrum. Through these interactions, students learn how the *Molecular Workbench* represents different forms of light, intensity, frequency, and energy.

---

[4] http://molit.concord.org/database/activities/283.html

Incorporated in the activity are several models that allow students to manipulate the energy of the photons, the intensity of the light source, the energy levels of the atoms, the simulation speed, and other parameters. Using these controls, students investigate ways in which light interacts with matter. Each instance of the *MW* model has different starting conditions, controls, and displays selected by the author to focus student inquiry on just a few relevant concepts. The student does not have to learn how to set up appropriate initial conditions and is not confused by unnecessary tools and displays.

Students use the models to explore how the energy of photons and the intensity of the light source may or may not affect photon absorption and emission, as well as how different types of atoms interact with various photons. With this knowledge, they are introduced to absorption and emission spectra and learn to read spectra as well as relate them to the excited states of atoms in the model. Finally, students analyze a model showing the transfer of energy from the photons to the atoms, moving them to an excited state and changing into kinetic energy, causing an increase in the temperature of the substance in the container. Students relate this model to how light can heat matter.

Pre-Post Test Comparisons

An examination of the effectiveness of the *Light and Matter Interaction* activity was conducted using pre- and post-tests. Students were asked to reason about the properties of light as well as the phenomena emergent from the interactions of light with matter. The identical pre- and post-tests consisted of three multiple-choice questions, two with associated open-ended justification questions for the choices they made, three open-ended questions, and five true/false questions about the properties of photons.[5] For each of the assessment items, item-specific rubrics were developed to score student responses. There were two, two-part items consisting of a multiple-choice response followed by an explanation; these two parts were scored separately. A two-point scale (0 or 1) was used for true and false questions and for multiple-choice questions. For open-ended questions there was either a three-point scale (0-2) or a four-point scale (0-3) depending on the level of complexity expected. All open response items were scored for content understanding. A total of 17 possible points could be scored on the test. The results did not count toward student grades. Statistical analysis was conducted using StatView® (Feldman, Gagnon, Hofmann, & Simpson, 1988). Two researchers scored all the open-ended questions independently. The inter-rater reliability based on scoring the three classes was 89.9%.

Paired group t-tests were performed on pre- and post-test scores for each class. The t-test revealed students' post-test mean total score to be significantly greater than their pre-test mean performance in each of the three classes.

Table I: Mean Test scores and Paired t-test results for three classes.

Class	**Mean Pre-test**	**Mean Post-test**	**Mean Diff.**	**DF**	**t-value**	**P-value**
1	**4.89**	**8.5**	**3.553**	**18**	**5.687**	**<.0001**
2	**5.1**	**10.15**	**5.031**	**15**	**10.584**	**<.0001**
3	**7.4**	**12.7**	**5.289**	**18**	**8.119**	**<.0001**

---

[5] The test and scoring rubric can be found at: http://molit.concord.org/database/activities/283.html#assessment

Analysis of Pre-Post Test Questions

Questions in the test were grouped into three categories that match the learning goals of the activity: 1) the properties of photons and the intensity of light; 2) the reaction of different substances to photons; and 3) the relationship of the absorption and emission spectrum to the excitation of an atom's electrons. Descriptions of questions and an analysis of student gains follow for each of these categories.

The Properties of Photons

Two questions addressed student conceptions of light. One focused on photon properties and the other on how the frequency of photons relates to absorption by atoms. The first question was a multiple-choice question on photon absorption and the second consisted of five true or false statements about photon properties.

The true-false items reveal that students appear to have learned from the activity that photons have no mass or charge, that they travel at the speed of light, carry energy, and move in straight lines. These questions can be used to assess students' conception of the properties of light prior to encountering the activity. The pre-test reveals that in spite of prior lectures and readings on this topic, students' mental models of photons were weak. This improved significantly, $p= <.0001$ after interacting with the models as revealed in a paired t-test analysis using responses of all students to just the multiple-choice question and the five true-false items. This is particularly important information because these students had completed the *MW*-based activity as a review after a photon-based treatment of light-matter interactions had already been covered in the classroom as reported by the teachers.

Students also showed an increased ability to reason about how the energy of light might relate to absorption or emission of the photon by specific atoms. Results from one multiple-choice question on this topic revealed a significant change in students' conceptions (p= .0007) based on a paired t-test pre-post comparison of scores of all students on this question. The responses required students to reason that a certain atom could absorb only a photon of a specific frequency, and that changing the frequency of the photon made it unable to be absorbed. On the pre-test, 15 % of the students chose the correct response, while on the post-test 43% selected the correct answer. Of interest was one of the distracters that probed a common misconception. This item would be selected if students believed that photons of the wrong energy could be absorbed by increasing the light intensity. On the pre-test 47% chose this answer; on the post-test 17% did so.

The Reaction of Different Substances to Photons

One of the major concepts covered in the activity was the three possible interactions of light with matter: a) light passes through matter; b) light is absorbed by matter; or c) light is scattered by matter. Models are provided that represent each case. Scattering is treated as absorption of a photon followed by prompt emission of a photon of the same energy in a random direction.

One open-ended question and two multiple-choice questions with associated justifications addressed these concepts. They all required students to transfer their understanding of light-matter interactions at the atomic scale to a range of observable macroscopic phenomena. In one of these questions, students were asked to think about a way in which light that is emitted from an excited atom might in turn interact with matter to produce light at a different energy level. The question states that mercury, when excited, emits ultraviolet light and challenges the student to come up with a way to convert the UV emitted by the mercury into visible light. Although fluorescence was not covered directly in the activity, the question was designed to reveal whether or not students could reason that the UV light could be absorbed by a substance and subsequently emit visible photons. This question invokes a fairly sophisticated series of connections and higher cognitive level thinking. Scores of all students for this question were significantly higher on the post-test than on the pre-test ($p= <.0001$).

Analysis of the pre-test revealed that 46% of students believed UV could be blocked to let visible light through, but did not reveal a mechanism for converting the UV into visible light; and 41% thought the only way to get UV light would be to change the light source itself and not use mercury. None of the students on the pre-test described a way to convert the UV light. In the post-test, 54% were able to reason that the problem could be solved by a coating that could absorb the UV emitted by the mercury and then emit visible photons when the excited atom drops to lower energy levels. Responses to this question showed a dramatic change. Initially, students did not use any reasoning based on light interacting with matter. In post-test responses, a majority of students reasoned about the interactions and provided a clear explanation about the correlation of atoms with multiple energy levels to light absorption and emissions.

Another multiple-choice question with an associated justification asked students to consider why yellow light emitted from a sodium lamp would make a blue object appear black. Again, this question requires students to explain how the atoms in the blue object interact with the photons emitted from the sodium lamp. The choices for the question had students consider whether the light is reflected, absorbed, or converted into another color. Paired t-tests revealed that students' scores on the multiple-choice part and the explanation improved significantly (p=.0065 and p=.0050, respectively). Analysis of student pre-test responses and justification indicated that a majority of students (68%) knew that blue substances absorb almost all visible photons falling on it except blue photons. However, of those students, only 30% could justify their choice without flawed reasoning such as blue objects absorbs light (incomplete), the absorbed light makes it black (incorrect), or the light is reflected (incorrect). On the post-tests, there was an increase of students choosing the correct response (85%), with 42% of the post-test justifications including accurate reasoning regarding the blue object absorbing all the photons emitted from the sodium lamp. Students in post-test responses were able to explain "blue objects absorb all the light falling on it except blue photons."

Another multiple-choice question and its associated justification required students to explain why glass is transparent. Each distracter is based on a common student misconception about transparency: light can pass through matter because the waves are either too long or too short; glass molecules line up to form channels; or light bounces off the glass. The correct answer is that there are no atoms or molecules that have excited states with excitation energies that correspond to visible photons. Scores on the multiple-choice and justification parts again showed significant improvement (p=<.0001 for each part separately).

On pre-test scores the answers were varied: 34% chose "light is not absorbed," 11% "light bounces off," 11% "light waves are longer than glass," 20% "light waves are shorter," 17% "glass molecules line up in channels." On the post-test, 77% chose that "light was not absorbed," 15% that it was reflected, and under 9% and 3%, respectively, for "light waves too small" or "light goes through channels." There was an apparent decrease in students' misconceptions. Pre-test justifications when provided most often just repeated one of the multiple-choice options. In the post-test, student justifications frequently included a variation on the following description: the glass does not absorb light because electrons in glass cannot jump to a higher energy level, and instead the photons pass through the glass.

Analyzing Absorption and Emission Spectra

To address the final learning goal, one question focused specifically on the concept that an emission spectrum can be used to identify the existence of certain elements. In this question, students needed to explain how it is possible for an astronomer to know what specific elements exist in the sun. This question asks students to apply what they learned about emission spectra from the activity and transfer it to a new situation to explain how scientists read the spectra from the sun. In the activity, students learn to relate the frequencies of absorbed or emitted light as represented in spectra to the excitation states of specific atoms. Students see how unique excitation states can be used as a "fingerprint" for identifying a specific atom.

Student answers improved significantly on this open-ended question (p=.0002). Pre-test answers included: "They see how the sun burns and how certain particles burn," "they know by the type of light emitted," and "because the colors that it [the sun] emits." Post-test answers included reasoning such as: "It is possible for astronomers to know this by comparing the spectra produced by sunlight to the spectra of elements they know,” “Each element produces a different type of light energy; astronomers can compare these to the light energy seen from the sun,” and “Each atom gives off certain wavelengths of light when in an excited state. Scientists can study this and compare to the sun’s light emissions.”

Conclusions and Implications

At the introductory level, light is almost always treated exclusively as a wave. Presumably, this choice is the result of following common practice and a reluctance to plunge into quantum mechanics because it is considered too difficult for beginning students. This practice leaves students no understanding of a wide range of important light-matter interactions based on atomic absorption and emission, such as transparency, color, spectra, and fluorescence. It also deprives them of the ability to reason about applications of photon-matter interactions such as light-emitting diodes, paint mixing, lasers, neon lights, incandescent light, colorimeters, and spectrometers.

Our approach avoids addressing quantum mechanics head-on by simply asserting that there are excited states of atoms and molecules that can interact with photons that carry energy. The interactions conserve energy and momentum, but permit conversions between photons, kinetic energy, and excited states. This links light to the temperature of the system, which can explain a variety of thermal effects of light.

This study demonstrates that these topics can be covered in a single class period. Students in our study not only acquired vocabulary and basic concepts, they also were able to transfer their understanding to new situations. After only a brief exposure to the materials, students in the test classes mastered much of the content, were able to apply their knowledge to new contexts, and made surprising intellectual leaps.

These gains can be attributed to both the unique *Molecular Workbench* software and the instructional design used. MW is unique in combining light-matter interaction rules with a molecular dynamics system designed for education. This software is necessary, but not sufficient; well-designed learning activities are also required. The activities feature learning that results from interacting with the model in order to answer contextualized questions. Students are guided to try different starting conditions and parameters in order to discover how the software works. Because the software is a reasonable approximation of reality, this inquiry builds a robust mental model of the real system—light-matter interactions.

This combination of a highly interactive, fast computational model that generates real-time visualizations and good inquiry-based instructional design can have broad application to science education. As seen in this study, innovative software and well-designed materials can foster learning that calls into question conventional assumptions about the content that introductory students can master.

References

Berenfeld, B., & Tinker, R. (2001). *Revolutionizing Science Teaching with Atomic Scale Models.* Paper presented at the National Education Computer Conference (NECC), Chicago,IL.

Bransford, J. D., Brown, A. L., & Cocking, R. R. (Eds.). (2000). *How People Learn: Bridging Research and Practice*. Washington, D. C.: National Academy Press.

Buckley, B., Gobert, J. D., Kindfield, A. C. H., Horwitz, P., Tinker, R., Gerlits, B., et al. (2004). Model-Based Teaching and Learning with BioLogica: What Do They Learn? How Do They Learn? How Do We Know? *Journal of Science Education and Technology, 13*(1), 23 - 41.

Clark, D., & Jorde, D. (2004). Helping students revise disruptive experientially supported ideas about thermodynamics: Computer visualizations and tactile models. *Journal of Research in Science Teaching, 41*(1), 1-23.

Clement, J. (2000). Model based learning as a key research area for science education. *International Journal of Science Education, 22*(9), 1041-1053.

Feldman, D., Gagnon, J., Hofmann, R., & Simpson, J. (1988). StatView (Version 1.03) [statistics]. Berkeley, CA: Abacus Concepts, Inc.

Feurtzeig, W., & Roberts, N. (1999). *Modeling and simulation in science and mathematics education*. New York: Springer.

Hallden, O. (1999). Conceptual change and contextualization. In W. Schnotz, S. Vosniadou & M. Carretero (Eds.), *New perspectives on conceptual change* (pp. 53-66). Oxford, UK: Pergamon.

Heering, P., & Osewold, D. (2007). *Constructing scientific understanding through contextual teaching*. Berlin, Germany: Frank & Timme, GmbH.

Horwitz, P., & Christie, M. (2000). Computer-based manipulatives for teaching scientific reasoning: An example. In M. J. Jacobson & R. Kozma (Eds.), *Innovations in science and mathematics education: Advanced designs for technologies of learning* (pp. 163-191). Hillsdale, NJ: Lawrence Erlbaum & Associates.

Jackson, S. L., Stratford, S. J., Krajcik, J., & Soloway, E. (1996). Making Dynamic Modeling Accessible to Pre-college Science Students. *Interactive Learning Environments, 4*(3), 233-257.

Johnson, E. (2001). *Contextual Teaching and Learning*. Santa Barbara, CA: Corwin Press.

Krajcik, J., Marx, R., Blumenfeld, P., Soloway, E., & Fishman, B. (2000). *Inquiry based science supported by technology: Achievement among urban middle school students*. Ann Arbor, MI: University of Michigan, School of Education.

Linn, M., Lee, H.-S., Tinker, R., Husic, R., & Chiu, J. (2006). Teaching and assessing knowledge integration in science. *Science, 313*, 1049-1050.

Pallant, A., & Tinker, R. (2004). Reasoning with atomic-scale molecular dynamic models. *Journal of Science Education and Technology, 13*(1), 51-66.

Parnell, D. (2000). *Tech Prep education: Contextual teaching works*. Waco, TX: CORD Communications.

Sears, S. (2002). *Contextual teaching and learning: A primer for effective instruction*. Bloomington, IN: Phi Delta Kappa Educational Foundation.

Slotta, J. (2004). The Web-based Inquiry Science Environment (WISE): Scaffolding Knowledge Integration in the Science Classroom. In M. Linn, P. Bell & P. Davis (Eds.), *Internet Environments for Science Education* (pp. 203-232): Lawrence Earlbaum Associates.

Snir, J., & Smith, C. (1995). *Constructing Understanding in the Science Classroom: Integrating Laboratory Experiments, Student and Computer Models, and Class discussion in Learning Scientific Concepts*. New York: Oxford University Press.

Tinker, R. (2007a). How do students learn from models? Case studies in guided inquiry. *@Concord, 11*(1), 14-15.

Tinker, R. (2007b). The science of atoms and molecules. *@Concord, 11*(1), 10-11.

Tinker, R., & Horwitz, P. (2000). Modeling Across the Curriculum: IERI Planning Grant. *National Science Foundation (REC-0089198)*.