

# Links between Dynamic Representations of Atomic-Scale Phenomena and Molecular Reasoning

**Dalit Levy**

The Concord Consortium  
dlevy@concord.org

**Robert Tinker**

The Concord Consortium  
bob@concord.org

## Abstract

This paper reports the results of a study aimed at exploring the advantages of dynamic visualizations for the development of better understanding of molecular processes. During the spring and the fall of 2006, six hundred students learned about phases of matter and phase change using TELS<sup>1</sup> online chemistry curriculum. The curriculum utilizes Molecular Workbench<sup>2</sup> dynamic molecular models of solid, liquid, and gas, and scaffolds the learners' interactions with these dynamic representations by embedded reflective prompts to help make and refine connections between observable phenomena and atomic level processes related with phase change. The explanations that students entered in response to pre/post assessments items have been analyzed using a newly developed scale for measuring the level of molecular reasoning. Results indicate that from pre-test to post-test, students make progress in their level of molecular reasoning, and are better able to connect intermolecular forces and phase change in their explanations. These findings add to our understanding of the benefits students gain from interacting with dynamic molecular models.

**Keywords:** visualizations, dynamic modeling, the molecular point of view, conceptual change.

## Introduction

Chemistry is often referred to as the “molecular” science. As such, students of chemistry are required to imagine scientific phenomena on an atomic-scale level and to employ a molecular point of view when explaining these phenomena. Typically, textbooks and classroom instruction include static visualizations and models that help students “see” the symmetries and structural factors involved in chemistry. Students are expected to make connections between these static visualizations and the observable phenomena, as well as to understand that the static representation is just one specific frame of the ever-changing dynamic molecular world. However, research suggests that when considering phases of matter and phase changes, students have difficulties both in connecting the observable and the molecular points of view (Smith, Wisner, Anderson, & Krajcik, 2006) and in realizing that molecules are in constant motion in solids, liquids, and gases (Pallant & Tinker, 2004).

Today's technology can provide ways for students to dynamically model scientific phenomena on the atomic- and even the nano-scale levels, and thus experience an otherwise inaccessible world (Xie and Tinker, 2006). Specially, student explorations of and interactions with atomic-scale dynamic models of solid, liquid and gas can lead to a better understanding of the

---

<sup>1</sup> TELS – Technology Enhanced Learning in Science, an NSF supported center headed by Prof. Linn (from UC Berkeley) and Dr. Tinker (from the Concord Consortium). See [telscenter.org](http://telscenter.org) for more details.

<sup>2</sup> The Molecular Workbench is developed at the Concord Consortium as a freeware. For details, see [mw.concord.org](http://mw.concord.org).

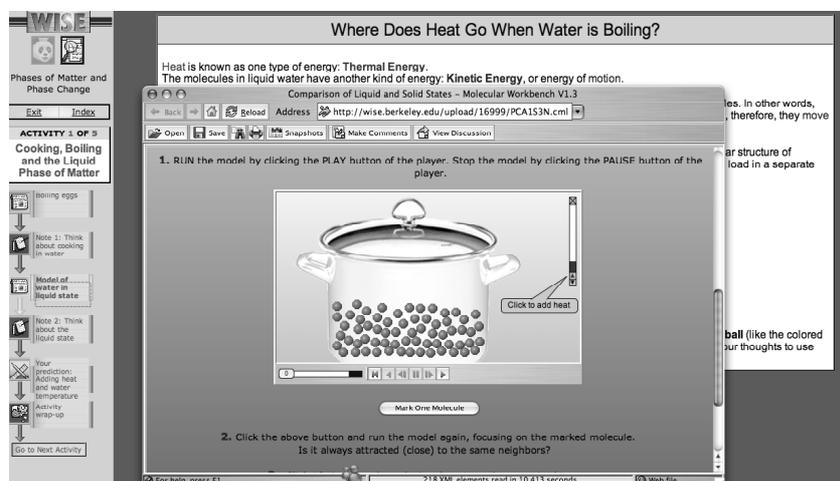
connections between atomic-scale events like overcoming an intermolecular force and those events that they can observe at the macroscopic scale like a cube of ice melting.

This study investigates the advantages of dynamic molecular visualizations for the development of better understanding of molecular processes of phase change. We define “Molecular Reasoning” (MR) as the ability to describe and explain scientific phenomena by referring to the atomic, molecular world (Levy, in preparation). Based on the assumption that a better understanding of molecular processes reflects a higher level of MR, this study asks: how do students improve in their ability to use molecular reasoning when explaining phase change, following the interaction with dynamic molecular visualization?

## Design and Implementation

The “Phases of Matter and Phase Change” project is one of more than twenty inquiry-based science curriculum units developed as part of the TELS center. The TELS units were created in the Web-Based Inquiry Science Environment (WISE, Linn, Clark and Slotta, 2003), and integrated novel visualization technologies from the Concord Consortium using The Molecular Workbench software (Xie and Tinker, 2006). By manipulating these visualizations, by interacting with the molecular models, and by reflecting on the interactions, students have the potential to develop a deeper conceptual understanding of the underlying chemical phenomena (Kozma, 2003).

The general goal of the “Phases of matter and Phase Change” project is to develop learners’ ability to employ a higher level of MR (molecular reasoning) when explaining daily phenomena involving phase change. The project contains five online web-based activities, which are usually completed by the students during five consecutive lessons.



**Figure 1. A dynamic molecular model embedded in the project’s first activity**

The TELS “Phases of Matter and Phase Change” project<sup>3</sup> was tested in eight public high schools during 2006. Overall, 600 students in grades 9-12 ran the project as part of their regular chemistry course. The online project lasted five lessons, typically over the period of one week, and the students were working in pairs, two students per one computer. The subject of phase change had not been taught before in these classes, but the students had previous experience with the atomic nature of matter. The implementation was accompanied with an extensive data

<sup>3</sup> <http://wise.berkeley.edu/student/topFrame.php?projectId=16999> (login requested).

collection, in order to create a rich documentation of the learning process, to gather a wide collection of learners' ideas, and to track changes in these ideas. Since the students were working in pairs, the gathered data represent collaborative thinking rather than individual ideas.

### Research data

As part of the study, we examined responses to a set of assessment items carefully designed to stimulate the thinking about the molecular world. These items included an open-ended part, in which students could use terms of their choice to describe a phenomenon or explain a behavior.

The assessment took place as an online test, when pairs of students typed their responses to the same test shortly before and immediately after running the whole project. The coding of four out of the ten items was done using the MR scale developed specifically for the aim of this study. Overall, we analyzed 1200 pairs of pre-test/post-test written descriptions and used the paired t-test to determine the significance of the change in MR level following the interaction with the project.

### The “Molecular Reasoning” scale for analyzing students’ explanations

The analysis began with examining different kinds of explanations students gave in response to the question “what happens to water molecules when a cube of ice is taken out of the freezer and left at room temperature?” in the pre-test. In responses like “the molecules expand and melt” (pair #89), “they spread apart” (#214), and “the water molecules start to move more instead of just rocking next to each other” (#241), students speak about molecules and thus reveal a certain level of molecular reasoning, while many other pre-test responses do not mention the molecular point of view at all (although the question directly points to describing molecular behavior). Still, even those responses that do mention molecular behavior, reveal different levels of molecular reasoning: those describing how the water molecules “expand” or “spread apart” when a cube of ice is taken out of the freezer seem to have a more static image of the molecular structure than those who explain how the molecules start to move faster and faster as the cube of ice melts.

The Molecular Reasoning scale (see Table 1) has naturally emerged from the students' explanations, and thus is grounded in the data. It is constructed of static, dynamic, and intermolecular levels of understanding in thinking about phases of matter and phase change. Thus, explanations that do not contain any traces of thinking in the molecular level are scored “0”, and those who do are scored “1”(static), “2” (dynamic), or “3” (intermolecular).

**Table 1. The Molecular Reasoning (MR) Scale**

Score	Description	Example
3	Dynamic MR (molecular reasoning), including correct description of the weakening of intermolecular forces	“When the ice cube is taken out of the freezer, the new temperature it experiences is higher than the temperature it was previously at. Thus, the energy difference is used to weaken the intermolecular forces that hold the water molecules together. So the molecules have less restriction of movement, making the water molecules take the liquid state”.
2	Dynamic MR (referring to molecular motion) OR understanding of the role of intermolecular forces in melting the ice	(i) “the water molecules start to move faster because of the energy flowing from the surrounding to the ice cube. As the water molecules start to move faster the ice cube starts to melt”. (ii) “they begin to absorb thermal energy and break free of their covalent bonds, thus they begin to change phase to water”
1	Static MR	“They become scattered because of phase change from solid -> liquid”.
0	No MR	“they heat up and thus change form a solid to a liquid”

## Results

The average MR score in the pre-test was 1.01, while the average MR score in the post-test was 1.55. The difference was found significant ( $p < .001$ ) in the paired t-test. This result shows that prior to using the TELS project and its embedded dynamic molecular models, most students were thinking in static terms only, while others didn't think about molecules at all (and were scored 0). After learning with the project, students clearly climbed above the static level of molecular reasoning, employing a more dynamic point of view. This change can be clearly attributed to the interaction with the Molecular Workbench models during the run.

Moreover, the MR scores distribute differently in the pre-test than in the post-test. The diagram in Figure 2 clearly shows a much fewer responses with the lower scores in the post-test (dark bars). It also shows a very low number of responses with the highest score in the pre-test, which means that the construct of "intermolecular forces" is not a part of the students' conceptual framework prior to learning with the TELS unit. The percentage jumps in the post-test, and the difference is clearly attributed to the visualization of intermolecular forces offered by the Molecular Workbench models used in the project.

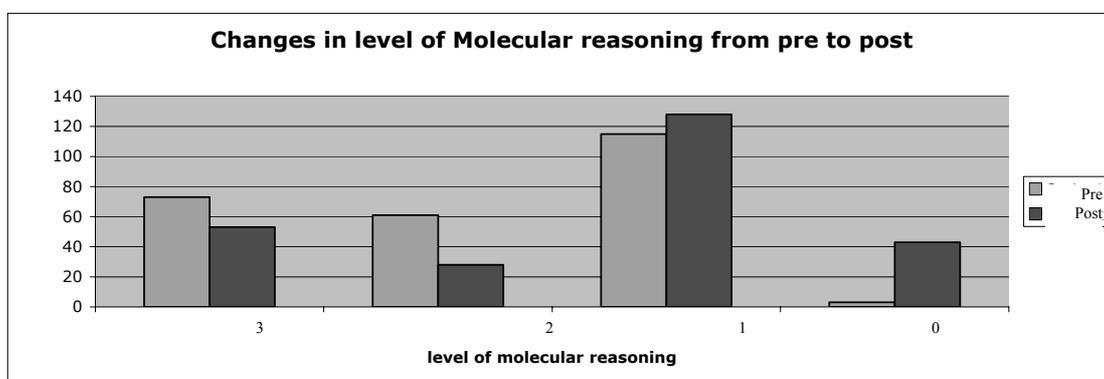


Figure 2. Distribution of MR level

## Summary

The behavior of large numbers of molecules each following individual rules of motion, and the related study of heat and phase change, is a complex subject for high school students to understand. The literature suggests some reasons for the difficulty, including the statistical understanding involved, the abstracted nature of thermodynamics as a theoretical system (Wilensky, Hazzard and Froemke, 1999), the students' inability to directly experience and observe these processes (Meir et al., 2005), and the separation of the micro-level phenomena from the macro-level phenomena (Dori and Hameiri, 2003). Our work points at an additional source of difficulty, namely the traditional instructional focus on static visualizations of the ever-changing dynamic molecular world.

The TELS "Phases of matter and phase change" project was developed in order to cope with these difficulties. Students learning with the TELS phase change project are given the opportunity to watch and follow what is otherwise too small to be seen and too fast to be traced, as well as to interact with these dynamic visualization, to reflect upon their interactions, and to improve their ability to explain phase-change-related phenomena. Using a newly constructed scale for measuring the conceptual change in terms of the level of molecular reasoning, our results show that the opportunity is more than a promise, and that students are indeed improving their molecular reasoning skills following the TELS experience.

## Acknowledgements

The work is supported by the NSF under the TELS grant. I deeply thank all of the TELS and MW researchers with whom I had so many meaningful hours of discussion.

## References

- Dori, Y.J. and Hameiri, M. (2003). Multidimensional analysis system for quantitative chemistry problems – Symbol, macro, micro and process aspects. *Journal of Research in Science Teaching*, 40(3), 278-302.
- Kozma, R. (2003). Material and social affordances of multiple representations for science understanding. *Learning and Instruction*, 13(2), 205-226.
- Levy, D. (in preparation). The Molecular Reasoning Scale: Static, Dynamic, and Intermolecular Levels of Thinking about Phase Change.
- Linn, M. C., Clark, D., & Slotta, J. D. (2003). WISE design for knowledge integration. *Science Education*, 87, 517-538.
- Meir, E., Perry, J., Stal, D., Maruka, S., and Klopfer, E. (2005). How effective are simulated molecular-level experiments for teaching diffusion and osmosis? *Cell Biology Education*: 4, 235–248.
- Pallant, A., & Tinker, R. (2004). Reasoning with atomic-scale molecular dynamic models. *Journal of Science Education and Technology*, 13 (1), 51-66.
- Smith, C. L., Wiser, M., Anderson, C. W., & Krajcik, J. (2006). Implications of Research on Children's Learning for Standards and Assessment: A Proposed Learning Progression for Matter and the Atomic-Molecular Theory. *Measurement: Interdisciplinary Research and Perspectives*, 4(1&2), 1-98.
- Wilensky, U., Hazzard, E., and Froemke, R. (1999). GasLab – an extensible modeling toolkit for exploring statistical mechanics. Paper presented at the *Seventh Annual European Logo conference EUROLOGO 99*, Sofia, Bulgaria.
- Xie, Q., and Tinker, R. (2006). Molecular dynamics simulations of chemical reactions for use in education. *Journal of Chemical Education*, 83, 77-83.