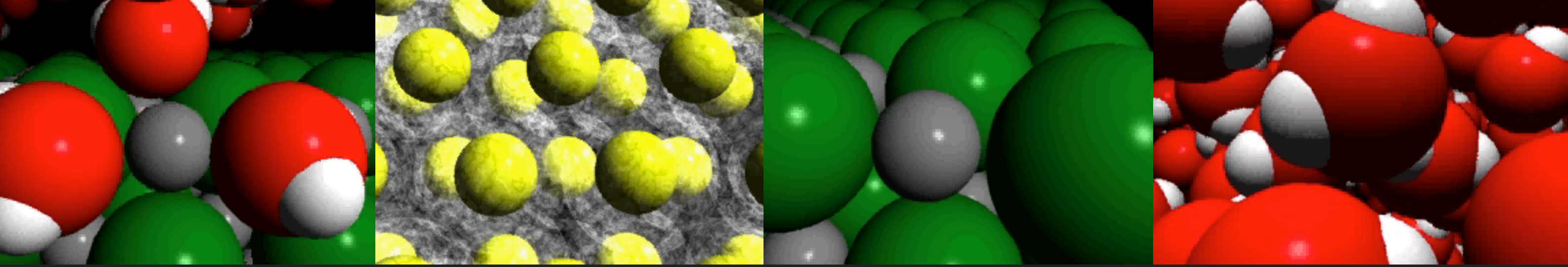


RESEARCH INTO PRACTICE

Visualising the molecular world for a deep understanding of chemistry

By Roy Tasker

INTRODUCTION

Why is chemistry so difficult?

A seminal paper by Johnstone (1982) offered an explanation for why science in general, and chemistry in particular, is so difficult to learn. He proposed that an expert in chemistry thinks at three levels; the macro (referred to as the observational level in this article), the sub-micro (referred to as the molecular level here), and representational (referred to as the symbolic level here). The observational level involves chemistry that is visible and tangible, incorporating what we can perceive with the senses. The molecular level of understanding consists of mental images that chemists use to imagine and explain observations in terms of atoms, ions and molecules. Observed phenomena and molecular-level processes are then represented in terms of mathematics and chemical notation at the symbolic level.

Figure 1 summarises these three levels for the chemical reaction that occurs when silver nitrate solution is added to solid copper. Dendritic silver crystals growing on the surface of the copper can be perceived at the observable level. At the molecular level an animation can portray the dynamic, but imperceptible, formation of silver atoms adhering to a growing cluster of silver atoms. The equation summarises the reaction at the symbolic level.

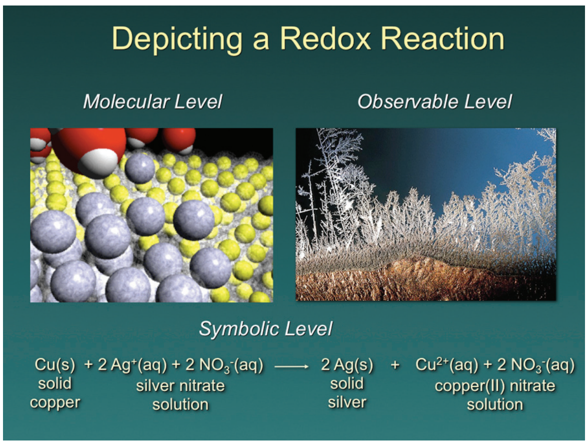


Figure 1: A redox reaction presented at the three thinking levels.

I first used these levels explicitly in my chemistry teaching in the late 1980s (Tasker, 1992), allocating different parts of the lecture stage to different levels (Figure 2). Reactions at the observable level were demonstrated on one side, often on an overhead projector, and an attempt to model the processes occurring at the molecular level on the other side. Only after these perspectives were these phenomena depicted at the symbolic level on the board. This three-level approach was reflected in the laboratory manual, study activities, and exam questions, to encourage students to integrate laboratory work and theory at each level. Other researchers have also recommended teaching at the different levels of thinking, and helping students to draw links between the levels (Tasker, Chia, Bucat & Sleet, 1996; Russell, Kozma, Jones, Wykoff, Marx & Davis, 1997; Hinton & Nakhleh, 1999).

Johnstone (1991) suggests that much of the difficulty associated with learning science occurs because "so much of teaching takes place … where the three levels interact in varying proportions and the teacher may be unaware of the demands being made on the pupils". Many students find it difficult to see the relationships between the levels (Kozma & Russell, 1997) and therefore, find it practically impossible to switch their thinking spontaneously between them. Understanding the relationships between the three levels does, however, vary from student to student, regardless of academic success (Hinton & Nakhleh, 1999). When students fail to see these relationships their knowledge is ultimately fragmented (Gabel, 1999) and many concepts may have only been learnt at a superficial level.

Gabel (1999) also suggests that problems arise because chemistry teaching has traditionally concentrated on the abstract, symbolic level and that teachers often have not considered the three levels in their own thinking. It is likely that teachers do not realise that they are routinely moving from one level to another during their teaching. However, presenting the three levels simultaneously to a novice is likely to overload his or her working memory (Johnstone, 1991; Gabel, 1999). If the levels are introduced together, numerous opportunities should be given to relate them, so that linkages are formed in the long-term memory.

WHY IS VISUALISATION AT THE MOLECULAR LEVEL SO IMPORTANT?

Nakhleh (1992) defined the term "misconception" as "any concept that differs from the commonly accepted scientific understanding of the term". There is convincing evidence in the literature (e.g. Kleinman (1987); Lijnse et al., (1990) and references therein) that many student difficulties and misconceptions in chemistry result from inadequate or inaccurate models at the molecular level. Moreover, many of the misconceptions are common to students all over the world, and at different educational levels. Lack of meaningful learning is demonstrated by the fact that many students can solve traditional-style chemistry problems without understanding the underlying molecular processes (Nurrenbern & Pickering, 1987; Nakhleh, 1993; Nakhleh & Mitchell, 1993; Niaz, 1995). The most important finding is that many misconceptions are extraordinarily resistant to change.

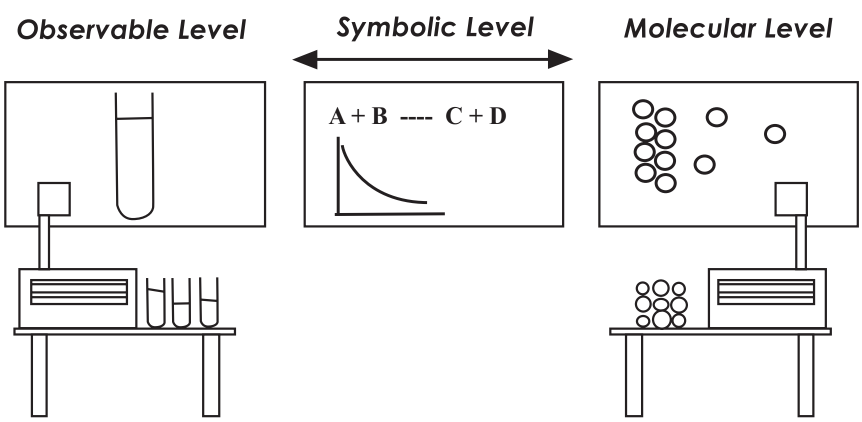


Figure 2: Dividing the lecture stage into the three thinking levels. This approach was also reinforced explicitly in the laboratory notes, tutorials and assessment.

HOW CAN WE HELP STUDENTS TO VISUALISE THE MOLECULAR LEVEL?

Until the early 1990s there was a shortage of resources that portrayed the molecular level so teaching and learning was restricted to the observable and symbolic levels, in the hope that students' mental models of the molecular world would "develop naturally". Students were then left to construct these models from the static, often oversimplified, two-dimensional diagrams in textbooks, or from their own imaginative interpretation of chemical notation—for example, did the formula "NaCl(aq)" mean that sodium chloride contained dissolved "NaCl molecules" in water?

Physical models (e.g. ball-and-stick) are static, and can be misleading models of substances like:

- solid sodium chloride, that does not have directional bonds or significant spaces between ions; and
- ice, where the distinction between intra-molecular and inter-molecular bonds is not clear because both are shown with sticks (albeit of different lengths).

However, physical models do provide a tactile, kinaesthetic dimension to appreciation of shape and angles. This can be more convincing than 2D representations (perspective or orthogonal) of 3D models on a computer screen, particularly without any previous experience with physical models. This can be likened to failure to navigate efficiently in virtual gaming environments without enough physical experience in the real world.

Since the molecular world is always dynamic it would be reasonable to assume that computer animations would be a more effective medium for depicting this world. However, animations often have a number of weaknesses, some obvious (use of 'artistic license' such as colour, and slow motion), some not so obvious but revealed through interviews with students, as described in the next two sections.

THE VISCHEM PROJECT—VISUALISING THE MOLECULAR LEVEL WITH ANIMATIONS

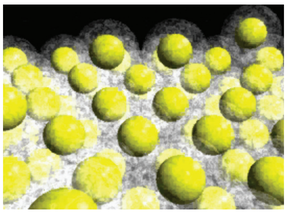
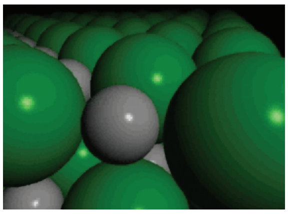
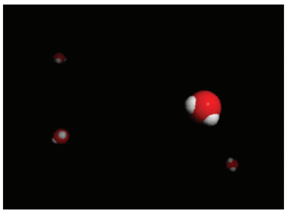
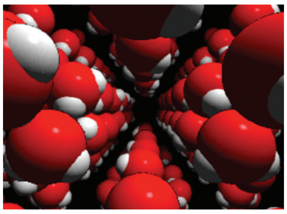
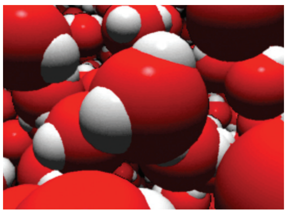
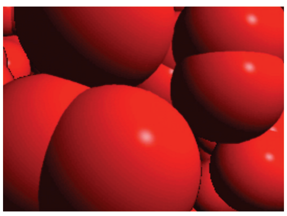
In the early 1990s the VisChem project was funded to produce a suite of molecular animations, depicting the structures of substances and selected chemical and physical changes (Tasker et al., 1996), to address student misconceptions identified in the literature. Table 1 lists many of the VisChem animations, and their targeted misconceptions from the educational literature. These misconceptions have been identified among students, from various age groups, regarding the nature of matter, molecular and ionic substances, aqueous solutions, and chemical reactions at the molecular level.

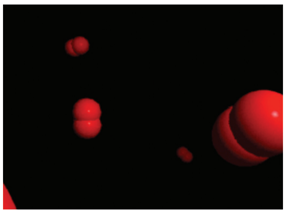
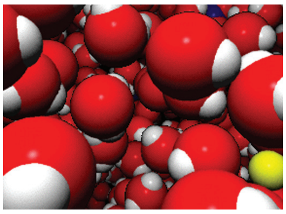
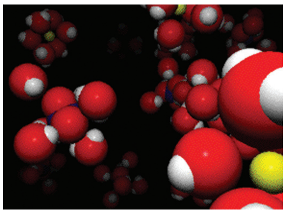
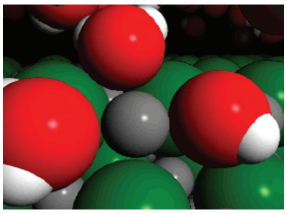
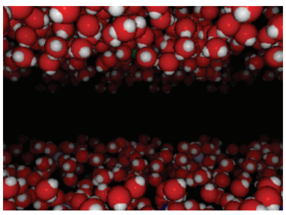
For instance, only VisChem animations portray the vibrational movement in solid substances (e.g. copper, sodium chloride in Table 1). This is important because this movement is correlated with temperature, and students need to understand this to interpret the significance of melting and boiling points in molecular-level terms.

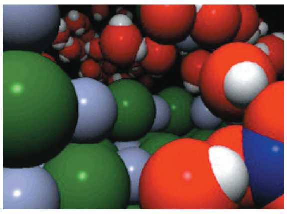
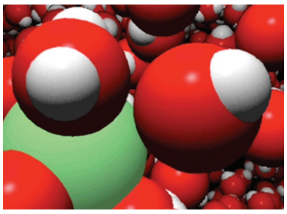
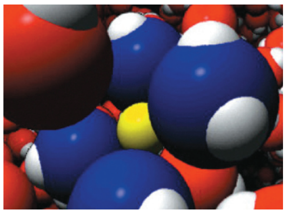
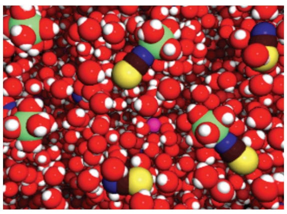
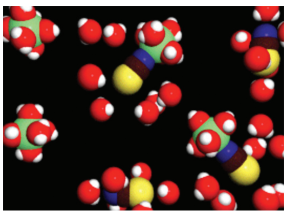
Many diagrams in textbooks depicting particles in the solid, liquid and gaseous states are misleading because the relative spacing between particles is inaccurate (e.g. Figure 1.7, p 7, in Brown et al., 2006). Little wonder that students develop poor mental models of states of matter. The VisChem animations are more accurate in this respect.

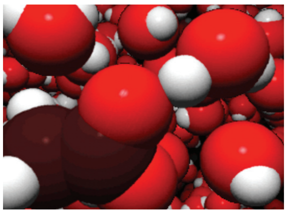
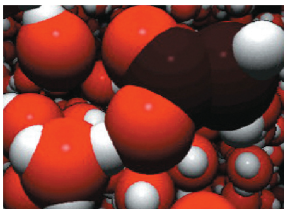
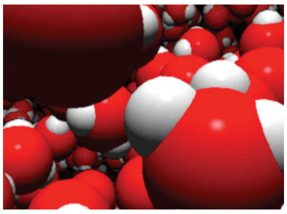
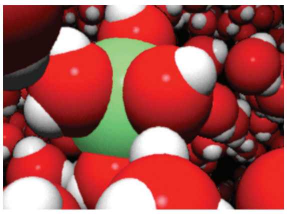
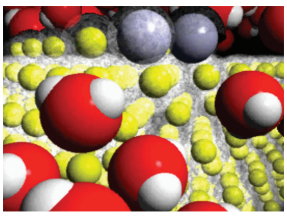
Few students have a 'feel' for the average distance between ions in a solution of a given concentration. VisChem animations portray ionic solutions at a concentration of about 1 mol/L, with ions separated from each other by, on average, about three water molecules (Table 1). This brings meaning to the magnitude of the number expressing molarity, in much the same way that people have a 'feel' for a length of one metre. Students are also encouraged to imagine dilution of a solution in terms of separation of ions by more water molecules.

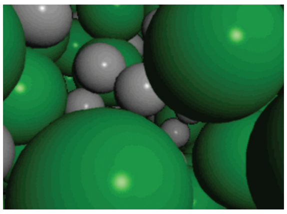
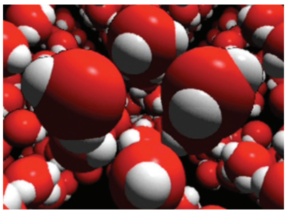
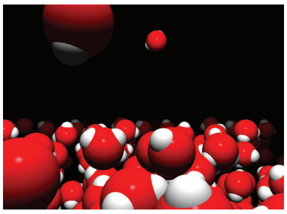
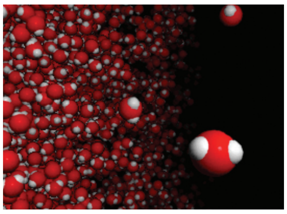
Table 1. List of selected VisChem animations, each with a key frame, description, and the misconceptions or difficulties addressed.

SELECTED FRAME	DESCRIPTION	MISCONCEPTIONS
METAL SOLID		
 Solid copper, Cu(s)	Close-packed copper atoms vibrate in an ordered lattice. Each atom is represented as a yellow copper(II) ion with its two electrons delocalised in a cloud.	Students have difficulty in conceiving of matter as multi-particulate. *Ben Zvi, Silberstein & Mamlok (1990)* Matter is conceived as static. *Novick & Nussbaum (1981)*
IONIC SOLIDS		
 Solid sodium chloride, NaCl(s)	Close-packed sodium and chloride ions vibrate as electrostatic forces hold them together.	There is a tendency to believe that there are molecules or discrete ion groups in ionic solids. *Taber (1994)* Students believe it is not possible to point to where the ionic bonds are unless you know which chloride ions have accepted electrons from which sodium ions. *Taber (1997)*
MOLECULAR SUBSTANCES		
 Gaseous water, $H_2O(g)$	The average distance between molecules in a gas is much larger than in the liquid and solid states.	Students have difficulty imagining empty space. Matter is conceived as continuous. There is no vacuum. *Andersson (1990)*
 Solid water (ice), $H_2O(s)$	We move into one of the hexagonal channels in the ice structure, look around at the vibrating molecules attracted together by hydrogen bonds, and then move back out of the channel.	Students confuse (1) intra-molecular bonds and inter-molecular bonds and (2) van der Waals forces and hydrogen bonds. *Levy Nahum, Hofstein et al. (2004)*
 Liquid water (ice), $H_2O(l)$	Water molecules move around, closely packed and attracted together by hydrogen bonds, with some molecules in clusters.	There is a tendency to suggest that ice is more densely packed than liquid water. *Griffiths & Preston (1992)* Students conceive of molecules in a liquid as being reasonably spaced such that it could be compressible. *Hill (1988)*
 Liquid oxygen, $O_2(l)$	Oxygen molecules in the liquid state move *almost* randomly with respect to one another.	Students conceive of molecules in a liquid as being reasonably spaced such that it could be compressible. *Hill (1988)*

 Gaseous oxygen, $O_2(g)$	Oxygen molecules moving quickly in space, occasionally colliding.	Students believe that there is little reduction in density when a liquid changes to a gas. *Pereira & Pestana (1991)*
AQUEOUS SUBSTANCES		
 Aqueous copper(II) nitrate (~1M), $Cu^{2+}(aq)$ + $2NO_3^-(aq)$ 	Hydrated copper and nitrate ions, and water molecules, in a 1:3:55 ratio, roam amongst the water molecules, with the occasional formation of a transient ion pair, followed by its dissociation. Solvent water molecules omitted in version below to show proximity of hydrated ions. Other VisChem animations show ~1M solutions of iron (III) nitrate, sodium nitrate, potassium thiocyanate, sodium chloride, and potassium fluoride.	Some students do not dissociate any ionic species in their representations of aqueous solutions. *Butts & Smith (1987)* Particles in aqueous solutions are not generally drawn touching. *Butts & Smith (1987)* Some students think that dissolved particles go into empty spaces inside water molecules. *Sequeira & Leite (1990)*
DISSOLVING		
 Solid sodium chloride dissolves $NaCl(s) \rightarrow Na^+(aq)$ + $Cl^-(aq)$	Skating over the surface of the NaCl solid the camera pauses to see the vibrating ions in the lattice. Then water molecules come tumbling down, hydrating the ions in a competitive 'tug-of-war' with electrostatic forces attracting the ions to the lattice.	There is a common inability to discriminate between dissolving and melting. *Haidar & Abraham (1991)* Students rarely acknowledge the role of the polar nature of the water molecule in the process of dissolution. *Butts & Smith (1987)* Students generally do not see dissolving as an interactive process but rather the automatic separation, then dispersal of solute molecules throughout the solvent. *Haidar & Abraham (1991)*
PRECIPITATION		
 Mixed aqueous solutions $Na^+(aq) + Cl^-(aq)$ + $Ag^+(aq) + NO_3^-(aq)$	At the molecular surface of the silver nitrate solution just prior to mixing with a sodium chloride solution being added from above. The mixing of solutions at the molecular level enables new combinations of ionic collision to occur.	Students cannot explain why the precipitate can form immediately when the solutions are mixed.

 Silver chloride precipitation $Ag^{+}(aq) + Cl^{-}(aq)$ $\rightarrow AgCl(s)$	In a solution containing silver, sodium, nitrate and chloride ions a silver ion and a chloride ion collide, and form a stable ion pair. Another ion pair joins, and the resulting cluster joins a growing crystal of silver chloride, with spectator ions in the background.	Students imagine that a precipitate is composed of 'molecules', each containing a neutral ion pair or group of ions.
COMPLEXATION		
 Water exchange on hydrated iron(III) $Fe^{3+}–OH_2(aq) + H_2O \rightleftharpoons$ $Fe^{3+}–OH_2(aq) + H_2O$	Exchange of a bonded water molecule with a nearby water molecule. Fe(III) ion represented by its van de Waals radius.	Students do not realise that water molecules in the first coordination sphere exchange with surrounding water molecules. This is a necessary first step in many complexation reactions.
 Copper(II) ammine complexation $Cu^{2+}(aq) + 4NH_3(aq) \rightleftharpoons$ $[Cu(NH_3)_4]^{2+}(aq)$	Successive substitution of water molecules with ammonia molecules, with Jahn Teller lengthening of axial bonds to coordinated water. Cu(II) represented by its ionic radius.	Students have difficulty imagining how a square planar complex can form in solution.
EQUILIBRIUM		
 Iron(III) thiocyanate complexation equilibrium $Fe^{3+}(aq) + SCN^{-}(aq) \rightleftharpoons$ $[Fe(H_2O)_5\ NCS]^{2+}$ 	Formation and dissociation of the isothiocyanatoiron(III) complex (each available as a separate animation) occurs at the same rate at equilibrium. Potassium and nitrate spectator ions are also present. The version below leaves out solvent water molecules and spectator ions to focus attention on the two reactions.	The use of everyday terms, "shift", "equal", "stress", "balance" when referring to equilibria can conjure up different visual ideas to students from those intended by the teacher. "Equilibrium" is seen as a static two-sided picture, and this can be unintentionally reinforced by misleading metaphors and analogies. Equilibrium is seen as oscillating like a pendulum, and Le Chatelier's stress-then-shift logic reinforces this misconception. *Bergquist & Heikkinen (1990)* Lack of awareness of the dynamic nature of the chemically equilibrated state. *Gorodetsky & Gussarsky (1990)*

ACID/BASE HYDROLYSIS		
 Acetate hydrolysis $CH_3COO^-(aq) + H_2O \rightarrow CH_3COOH(aq) + OH^-(aq)$	An acetate ion removes a proton from a water molecule, with some difficulty, to form an acetic acid molecule and a hydroxide ion.	A base is something which makes up an acid. *Hand and Treagust (1988)*
 Dissociation of acetic acid $CH_3COOH(aq) + H_2O \rightarrow CH_3COO^-(aq) + H_3O^+(aq)$	An acetic acid molecule donates a proton to a water molecule, with some difficulty, to form an acetate ion and a hydronium ion.	An acid is something which eats material away or which can burn you. *Hand and Treagust (1988)*
 Autoionisation of water $H_2O + H_2O \rightleftharpoons HO^- + H_3O^+$	Amongst the bustle of water molecules two come together and exchange a proton, forming a hydronium ion and a hydroxide ion.	Students have difficulty imagining how pure water can contain any hydronium ions and hydroxide ions.
 Iron(III) hydrolysis $Fe\text{-}OH_2^{3+} + H_2O \rightarrow Fe\text{-}OH^{2+} + H_3O^+$	One of the coordinated water molecules on iron(III) loses a proton to a solvent water molecule. The charge density of the metal ion increases the acidity of the coordinated water molecule through polarisation.	Students have difficulty understanding how metal ions (without hydrogen atoms) can produce hydronium ions.
REDOX REACTION		
 Reduction of silver(I) by copper $Cu(s) + 2Ag^+(aq) \rightarrow Cu^{2+}(aq) + 2Ag(s)$	Hydrated silver ions migrate towards the copper surface. Electron cloud moves onto the silver ions to form atoms, with concomitant release of copper ions from the metal lattice. Both anodic and cathodic sites are represented.	Students have a "reluctance" to perceive or represent chemical reactions as multi-particulate. *Ben-Zvi, Eylon & Silberstein (1987, 1990)* Students "cannot grasp the interactive nature of a chemical reaction". *Ben-Zvi, Eylon & Silberstein (1987)*

PHYSICAL CHANGES		
 Sodium chloride melting $NaCl(s) \rightarrow NaCl(l)$	To show the difference between dissolving and melting we see the total energy of the ions in solid NaCl rise until the structure collapses to the liquid state.	Students believe that there is a significant reduction in density when a solid melts. *Hill (1988)*
 Ice melting $H_2O(s) \rightleftharpoons H_2O(l)$	Starting within the ice structure the camera moves down to the molecules on the lower surface prior to melting. The total energy rises until the structure collapses to the liquid state.	There is a tendency to suggest that ice is more densely packed than liquid water. *Griffiths & Preston (1992)*
 Evaporation of water $H_2O(l) \rightleftharpoons H_2O(g)$	Starting within the liquid water the camera moves up to the surface. Molecules break away, with some difficulty, and some return. More leave than return.	Students believe that there is little reduction in density when a liquid changes to a gas. *Pereira & Pestana (1991)* Students believe that molecules increase in size when moving from solid to liquid to gas. *Gabel & Samuel (1987)* Students believe that intramolecular forces are broken in phase changes. *Ben-Zvi, Silberstein & Mamlok (1990)*
 Inside a boiling water bubble $H_2O(l) \rightleftharpoons H_2O(g)$	Moving through the water molecules in the liquid bubble wall, we suddenly break into the gaseous interior of the bubble. Some of the bubble wall can be seen in the background.	Bubbles in boiling water are made up of "heat" or "air" or "oxygen and hydrogen". *Osborne and Cosgrove (1983) & Bodner (1991)* Melting and boiling of molecular compounds are processes in which covalent bonds within molecules are broken. *Sleet (1993)*

These animations are freely available for non-commercial purposes on the Scootle site at **http://tinyurl.com/VisChemOnScootle**

They have also been incorporated into a range of multimedia programs associated with university-level chemistry textbooks (Jones & Tasker, 2002; Tasker, 1999; Tasker, 2001; Tasker, 2004; Tasker, Bell, & Cooper, 2003).

The animations portray substances, some in different states of matter, some undergoing physical changes, and some involved in common chemical reactions, as summarised in Figure 3. All the building blocks—individual atoms, molecules, ions, and hydrated ions—are available as separate animations for use as 'symbol legends'.

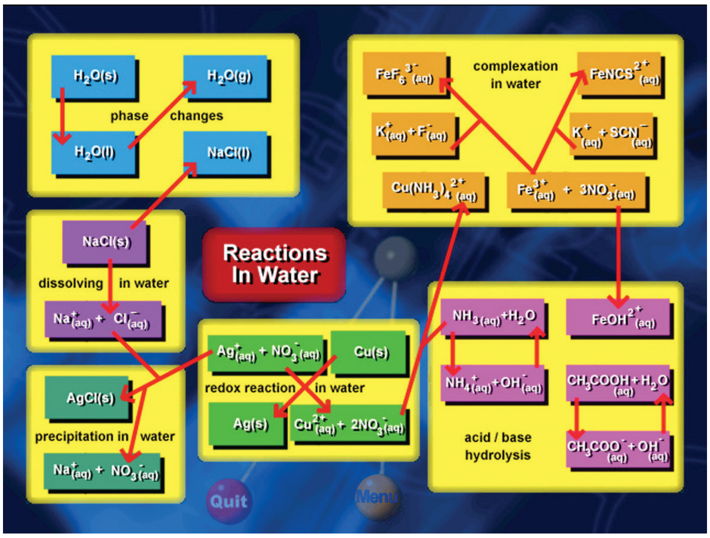


Figure 3: Each substance and solution shown above is depicted in a VisChem animation. The physical and chemical changes shown with arrows are also animated.

Most molecular-level processes involve competition between conflicting processes. Atkins (1999) has recommended that this is one of the most important 'big ideas' that we should communicate to students. Examples of this theme in VisChem animations include the competition for a proton between a base, like ammonia, and a water molecule (Figure 7); and between lattice forces and ion-dipole interactions when sodium chloride dissolves in water (Figure 8).

The animations were designed to be useful models of substances and processes at the molecular level. The challenge was to balance the often-competing demands of:

- scientific accuracy – such as very little space between adjacent molecules in the liquid state; complicated internal molecular bond vibrations; and the diffuse nature of electron cloud surfaces of atoms
- 'artistic license' required for clear communication – such as depicting slightly less than realistic crowding in the liquid state to enable visibility beyond the nearest molecules; the absence of internal molecular bond vibrations to reduce the degree of movement; use of reflective boundary surfaces on atoms at their van de Waals radii; and greatly reduced speed of molecules in the gaseous state
- technical computing constraints on rendering times and file size – such as the close-up view to limit the number of moving objects to be rendered; and the depiction of non-trivial events in minimum time to reduce the number of animation frames.

Animations of the molecular world can stimulate the imagination, bringing a new dimension to learning chemistry. One can imagine being inside a bubble of boiling water, or at the surface of silver chloride as it precipitates, as depicted in Figures 5 and 6 respectively.

Like all molecular-level animations, VisChem animations can also communicate misconceptions about processes at this level. They all convey the clear perception of 'directed intent'

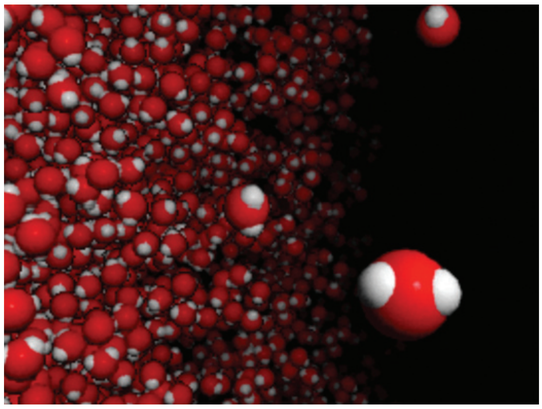


Figure 5: A frame of the VisChem animation that attempts to visualise gaseous water molecules 'pushing back' the walls of a bubble in boiling water.

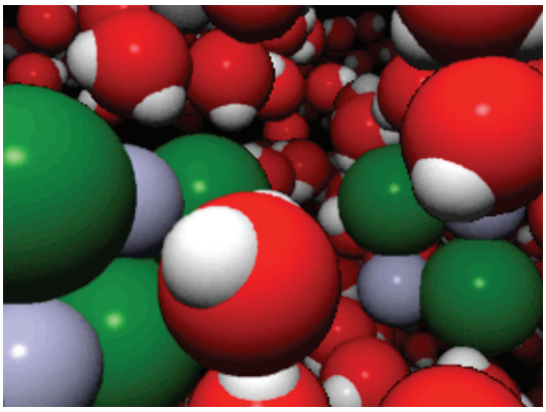


Figure 6: A frame from another VisChem animation that depicts the precipitation of silver chloride at the molecular level.

in molecular-level processes, instead of a more scientifically-accurate, probabilistic behaviour, governed by thermodynamics and kinetics.

We discovered this flaw during interviews with students. For example, one student thoughtfully drew this to our attention in the animation portraying silver chloride precipitation:

> *"This animation...shows water molecules...sort of carrying this structure [AgCl ion pair] along…like a bunch of little robots…The animation depicts something that…I think really happens by chance, as a very deliberate and deterministic sort of process and I think that's slightly misleading…Surely it must be possible to make it look less deliberate, less mechanical, maybe by showing...the odd one or two going into the structure but not all of them."*

The reasons that animation frames are not usually 'wasted' on depicting unsuccessful encounters (the majority) are related to the technical imperative to reduce rendering times, and to minimise file size to enable rapid delivery over the web. However, we need to explicitly point out to students that this is a form of 'artistic license', and can be likened to the conventional use of a chemical equation to describe a reaction, rather than to list all the steps in the reaction mechanism.

In contrast to choreographed animations, theory-driven simulations (e.g., Odyssey by Wavefunction, Inc.; see wavefun.com) offer a more accurate depiction of structures and processes at the molecular level. However, a limitation of simulations is that they often do not show key features of molecular events clearly because they occur only rarely (sometimes taking years in the slowed-down timescale used), at random, and usually with intervening solvent molecules blocking the view. Clearly simulations and animations should be used to complement one another.

Finally, we have found that if visualisation is to be taken seriously by students as a learning strategy, it is essential that they are encouraged to practise their new skills with new situations, and

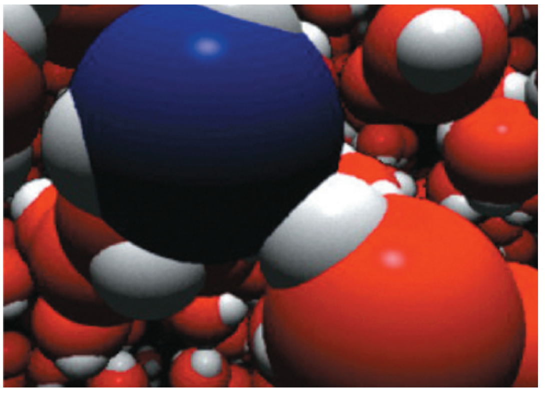


Figure 7. Frame from a VisChem animation showing the 'tug-of-war' between an ammonia molecule and a water molecule for one of its protons.

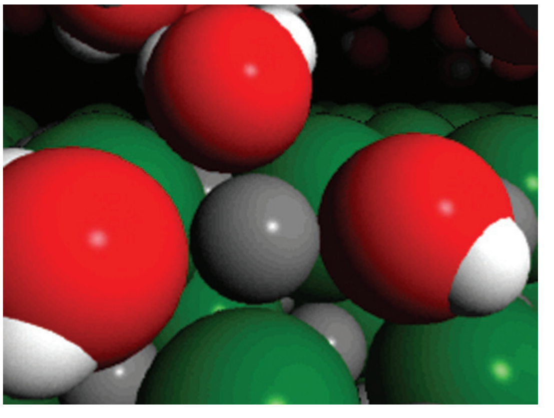


Figure 8. Frame from a VisChem animation showing the hydration of a sodium ion on the surface of sodium chloride, despite strong attractive forces from the rest of the lattice.

assess their visualisation skills in one's formal assessment. In addition to questions that probe qualitative and quantitative understanding of concepts at the symbolic level, we need to design questions that require students to articulate their mental models of molecular-level structures and processes.

CONCLUSION

The need for a chemistry student to move seamlessly between Johnstone's three 'thinking-levels' is a challenge, particularly for the novice. Our work in the VisChem project indicates that animations and simulations can communicate many key features about the molecular level effectively, and these ideas can link the laboratory level to the symbolic level. However, we have also shown that new misconceptions can be generated.

To use animations effectively, we need to direct our students' attention to their key features, avoid overloading working memory, and promote meaningful integration with prior knowledge. We can do this by using constructivist learning designs that exploit our knowledge of how students learn. A demonstration of our VisChem learning design can be seen at **https://www.youtube.com/watch?v=I7Hrj0hiWS8** .

'Scarring' misconceptions are those that inhibit further conceptual growth. To identify these misconceptions we need a strategic approach to assist our students to visualise the molecular level, and assess their deep understanding of structures and processes at this level.

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