Class:

**Visual Quantum Mechanics** 

LUMINESCENCE It's Cool Light!

# ACTIVITY 7

# Applying Potential Energy Diagrams to Solids

### Goal

We continue to use the potential energy diagram as a representation of atoms. By bringing these "atoms" close together we see how spectrum from solids are created.

For the model of the atom to represent solids it must include many atoms which are relatively close together. In a solid these atoms interact with each other. The result of those interactions create the properties that we associate with solids. They also create the conditions that enable some solids to emit the light that we have seen

To understand how interacting atoms in solids lead to the broad spectrum of LEDs and other solids we will use the *Energy Band Creator*.

Open the *Energy Band Creator* computer program.

Use the program to create a single potential energy diagram that has a width of 0.1 nm and a depth of - 400 eV.

Use the program to determine the allowed energies for this potential energy diagram.

Sketch below the allowed energy values for the single potential energy diagram as displayed by the program.

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To represent two atoms in this space, add a second potential energy diagram. In the Regular Solid folder found on the bottom of the screen, type "2" in the box labeled Number of Atoms and set the Separation distance to 0.5 nm. Keep the same depth and width as before.

Find the allowed energies for these two potential energy diagrams and sketch them in the space below.

? How do the allowed energies of the two potential energy diagrams placed together compare with that of an individual diagram?

Now move these potential energy diagrams closer together. Keeping the depth and the width of the potential energy diagrams the same, decrease the separation to 0.15 nm.

Find the allowed energies for these potential energy diagrams and sketch them below. (Use the zoom-in function of the program to get a closer look at the allowed energies.)

? How do the allowed energies of the two potential energy diagrams change when they are brought closer?

We have seen what happens to the allowed energies when two atoms represented by potential energy diagrams are brought close together. Now explore what happens when the number of "atoms" increases.

Use the program to increase the number of potential energy diagrams to the number assigned by the instructor by keeping the depth, width, and separation distance constant. Use the **Update Graph** button to determine the allowed energies in each case.

Describe, using words and sketches, what happens to the allowed energies as the number of potential energy diagrams increase to the assigned number. Again, you will need to use the zoom function to look closely at each set of energy levels.

Compare your results with other students who were assigned different numbers. The resulting discussions should focus on answering the following questions:

- ? How are the allowed energies in your diagram similar to the others?
- ? How are they different?

The atoms in a solid are relatively close together as in the diagrams we just explored. For instance, the 15 potential energy diagrams are a representation of a 15 atom solid. Such a solid is incredibly smaller than a real solid. For example, the small solid inside an LED has over 10<sup>23</sup> atoms. However, our less dense solids can give us some idea of how the energies of several closely spaced atoms differ from the energies of isolated gas atoms.

Describe the similarities and differences between the allowed energies of atoms in a solid and those of a gas.

The trend that we saw when we increased the number of atoms continues for very large numbers of atoms in a solid. The energy level diagram for such a solid is shown in Figure 7-1. When the number of atoms increases, the energies merge into groups with no energies allowed between these groups. These allowed energy groups are called *energy bands* and are separated by *energy gaps*.



Figure 7-1: Energy diagram with a very large number of solid atoms. Only the upper two energy bands are shown.

Electrons with total energies represented near the top of the energy diagrams are relatively energetic. They are not firmly attached to their respective atoms and can wander about freely throughout the solid. These electrons have energies in the *conduction band*. Notice from Figure 7-1 that the conduction band is located above the individual potential energy diagrams that make up the solid (to represent that the electrons with these energies can move from one atom to the next inside the solid) but are inside the two potential energy diagrams found at the edges (to represent that the electrons with these energies are still bound to this solid).

Recall that the values of the allowed energies for an electron are negative because the electron is bound to the atom. Electrons in the conduction band have relatively small negative values of energy. Other electrons have lower total energies. These electrons are bound to their respective atoms more strongly. These electrons are associated with the next lower energy band that is called the *valence band*.

Figure 7-1 illustrates the energy bands which have the greatest energy and which are important in explaining the physical properties of a solid. Solids also have allowed energies in addition to those found in the conduction and valence bands. Electrons with these lower allowed energies, however, do not influence the overall solid's properties in which we are interested.

These energy bands are similar to the bands that you needed to create to explain the spectrum of the LEDs. When you created those bands, you needed to do it to explain your observations. Now, we see that a relatively simple model of the atom leads to the same conclusions — the energies in solids are grouped in bands with energy gaps between them.

As a brief review Figure 7-2 shows how energy bands and gaps explain the continuous spectrum of luminescent objects.



Figure 7-2: Energy bands and energy gaps can explain the spectra of luminescent objects.

Our simple model of representing atoms with squared off potential energy diagrams is not as complex as a real atom. However, it is able to explain our observation of spectra.

At this time we have concluded that energy bands and gaps are consistent with our observations of the spectra which is emitted by solids. We have not, however, explained differences in the various types of light emission. Our model does not allow us to understand why some solids glow in the dark and others do not. So, we need to take the model one step further and look at additional features. We do that in future activities.

# Appendix

### Energy Bands, Energy Gaps, Conductors & Insulators

If you have studied either the conduction of electrical or thermal energy in solids, you probably have guessed that the name "conduction band" is related to conductors and insulators.

The electric current that flows through a solid consists of electrons with energies associated with the conduction band. Solids that conduct heat or electric current (called *conductors*) will have many electrons with energies associated with the conduction band. Solids that do not readily conduct heat or electric current (called *insulators*) will have few electrons with energies in the conduction band. Thus, the electrons for insulators are found mostly in the valence band. Solids that are good conductors will have many electrons in the valence band because these materials have enough electrons to fill the valence band and many left over to occupy the conduction band.

In addition to the difference in the number of electrons found in their respective conduction bands, conductors and insulators also differ in the size of their respective energy gaps. For conductors, the two bands either overlap or are so close together that electrons from the valence band can easily acquire enough energy to move to conduction band. Insulators, on the other hand, have energy gaps that are so large that thermal or light energy would not be sufficient for electrons to move to the conduction band from the valence band.