Cluster Solids: Ionic, Covalent, or Both?

We all want faster computers, more powerful solar cells, and more sources of energy that don't contribute to pollution. In order to develop these technologies, scientists and engineers research and create new materials. Current work focusing on a new type of solid, called a cluster solid, is allowing scientists to create materials with precise magnetic and electronic properties. Because of the control scientists have over these properties, cluster solids may be part of a supercomputer or highly efficient solar panel someday.

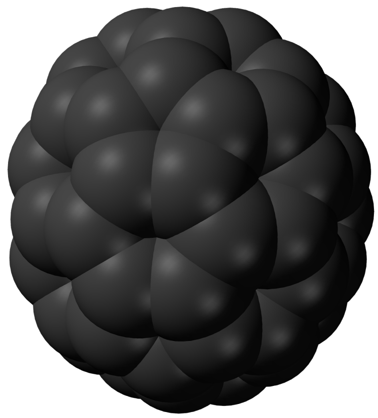

Figure 1. Fullerene. Space filling model of fullerene showing the connections between atoms of carbon. *Source:* Wikimedia Commons.

Cluster solids are materials that are made up of really big particles called **cluster units.** These cluster units are composed of many atoms held together by covalent or ionic bonds (or a mixture of both), depending on the identity of the cluster unit. Cluster units are capable of bonding to each other like individual atoms do in ionic solids by transferring electrons. They can be a full order of magnitude (up to 10 times!) bigger than an atom. For example, **fullerene** or **C_{60}** (**Figure 1**) is a cluster unit made up of 60 carbon atoms organized in the shape of a soccer ball. Fullerene cluster units are one nanometer in diameter—almost four times bigger than the diameter of a single carbon atom, as shown in the figure. To get an idea of how those compare think about a tenth grader and a two story building. If an atom were the size of a tenth grader, a fullerene cluster unit would be as big as a two story building! The difference in size between cluster units and atoms is enormous and leads to some of their interesting properties.

Cluster solids can be made up of many different types of cluster units. Depending on the identity of the cluster units the resulting cluster solids have varying amounts of magnetism and varying abilities to conduct electricity. This means that their magnetism and electrical conductivity are "tunable"—they can be controlled by varying the components of the cluster solid.

Scientists at Columbia University created a variety of cluster solids to investigate their tunable properties. To make the cluster solids, they first created several different transition metal-containing cluster units. Each of these transition metal-containing cluster units was combined with C_{60} cluster units to make a different cluster solid. They found that an ordered ionic structure formed in all of these cluster solids, but the exact arrangement of the cluster units and the properties that resulted varied depending on the atoms in the transition metal cluster units. For example, one difference between these solids is that they combine in different ratios with C_{60} depending on how many electrons were transferred. This is similar to the way that calcium combines with two chlorides to make $CaCl_2$, but sodium only combines with one chloride to make NaCl. When a nickel-containing cluster unit was mixed with C_{60}, it made a 1:1 structure that is analogous to the structure of sodium chloride, which contains one sodium ion for every chloride ion (see **Figure 2**).

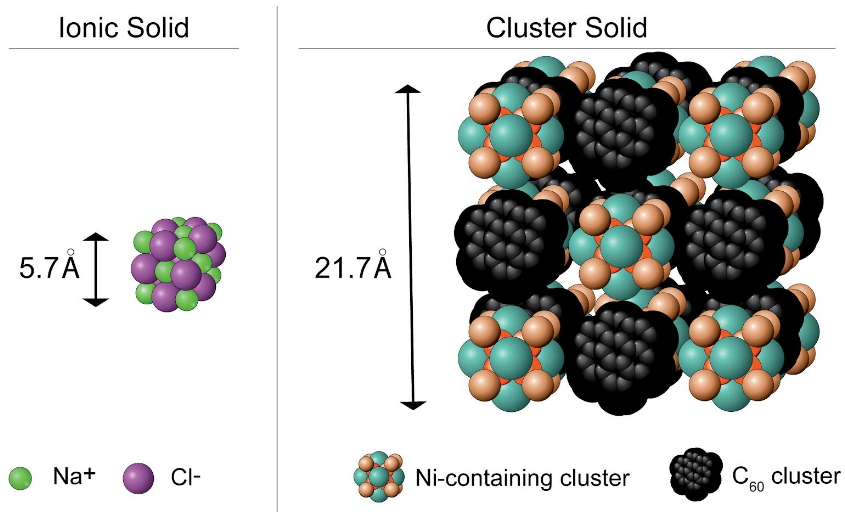

Figure 2: A Comparison of Two Crystals. There are similarities and differences between a typical ionic crystal (left) and a cluster solid (right).

Within a layer, the different types of cluster units are bonded together ionically, where a transition metal cluster gives electrons to C_{60}. The layers are held to one another by non-ionic intermolecular forces. So this type of cluster solid is in some ways similar to both an ionic solid and a molecular solid: inside the layers, there are cluster units held together in a way similar to ionic solids; by contrast, the layers are held together by intermolecular forces, similarly to molecular solids. This information is summarized in **Figure 3.**

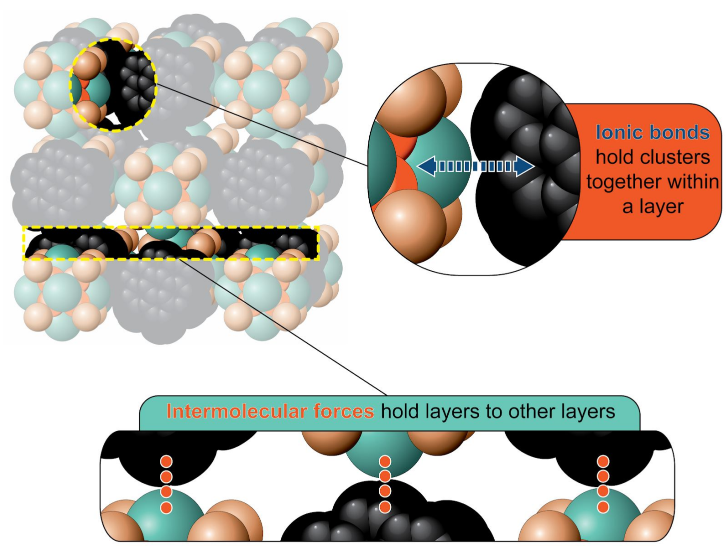

Figure 3. Bonding within a Cluster Solid. Ionic bonds hold transition metal clusters to C_{60} clusters within a layer, while intermolecular forces hold layers together.

When scientists develop new materials for industrial use, they need to be able to control their properties. Each cluster solid created by the scientists at Columbia University had different magnetic properties depending on the transition metal in the transition metal-containing cluster unit. Some of the cluster solids also had interesting electronic properties, which is significant because chemists are constantly developing new materials for electronic applications, in order to make better solar cells, computers, and energy storage systems. However, to make these newly developed materials useful, they have to be well characterized—we have to know which atoms are where and how they change the electronic properties of the material. This work uses clusters to make solids with "tunable" properties, so researchers can develop materials they can control and fine-tune for these important applications.

Reference

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BiteScientist Profiles

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