

Mathematical Beading as Molecular Analog Computation: An Example from Beaded Sierpiński Buckyball

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Abstract

Mathematical beading can be viewed as a process of analog computation. Combining the physical properties of beads, the figure-eight stitch and suitable algorithms, an approximate three-dimensional molecular structure for a molecule can be created through beading. The hard-sphere repulsion among beads and fishing strings that hold the whole structure together effectively mimic repulsion and attraction in the microscopic molecules. We demonstrate these ideas by creating a bead model of two-layer Sierpiński buckyball fused by 60 buckyballs.

Introduction

In previous Bridges conferences, we showed that mathematical beading can be used to model three-dimensional structures of nanoscale fullerenes and graphitic structures, substances composed of trivalent sp^2 -bonded carbon atoms [1, 2, 3]. As an art form, beading has been around for thousands of years and has gone far beyond the stringing of simple necklaces. Beadwork can take the form of jewelry, accessory, personal adornment, bag, sculpture, etc. Many of beadwork techniques such as figure-eight stitch, loom and off-loom weaving, and peyote stitch have their origins in different regions of the world. Particularly, creating three-dimensional bead sculptures using the figure-eight stitch is quite popular in oriental countries.

We demonstrated that, by using the figure-eight stitch, we can create not only faithful, but also aesthetically pleasing bead models of many different nanoscale fullerene structures. We believe that these vividly colored bead models enable us to visualize the invisible nanoscale molecular world in a new perspective. Here in this communication, we wish to point out that the success of bead models for modeling molecular structures is deeply rooted in the surprising connection to the basic chemical bond theory.

Combined with the algorithmic rules such as the spiral codes for cage-like fullerenes, mathematical beading can be viewed as a kind of analog computation. The result of computation gives an approximate three-dimensional electron density profile of the corresponding molecule. To demonstrate the power of mathematical beading for modeling three-dimensional structures of complicated molecular models, we describe a hypothetical two-layer Sierpiński buckyball that contains 4500 carbon atoms through fusion of 60 buckyballs [4, 5].

Valence sphere models and molecular analog computation

In this section, we want to show that the bead model of a molecule can be viewed as a physical realization of the valence sphere model of chemical bond. The valence sphere model, also called the tangent sphere model, was originally proposed as an approximate molecular orbital theory by the renowned American quantum

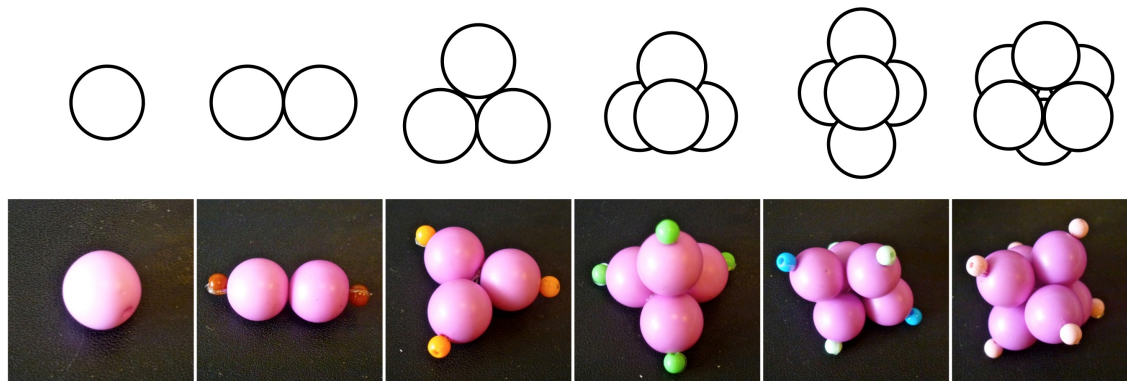


Figure 1: *Bead valence sphere models of single atom, and two, three, up to six valence electron pairs.*

chemist, G. E. Kimball [6], in the 1950s. Its connection to the Lewis electron-pair model was later seized upon by H. Bent and served as a focal point for many of his works on chemical bonding [7].

Valence electron pairs in a molecule are approximated by uniform and non-overlapping charge spheres with diameters equal to the electrons' de Broglie waves in the valence sphere model. The use of non-overlapping spheres ensures the Pauli exclusion principle, which requests that electron pairs can never occupy at the same place at the same time. The balance between electron-electron repulsion among charge spheres, owing to Coulomb's law and the Pauli principle, and nucleus-electron attraction provides the reason for the formation of molecules from electrons and nuclei.

Very interestingly, bead models are possibly the only molecular models that can account for these two contributions responsible for molecular formation. The spherical beads exactly mimic valence shell electron pairs. The point located at the center of several neighbored beads represents the site of an atomic core. The tension of the fishing strings or rubber bands simulates atomic-core/electron-pair attraction. In Figure 1, we show the equilibrium shape for molecules with one to six valence electron pairs. By combining hard spheres in different ways, we can create diagonal, trigonal, tetrahedral, trigonal bipyramidal, and octahedral arrangements. We can see that the interaction among hard spheres in bead models is fully capable of accounting for the saturation and directional character of chemical bonding of different coordination numbers.

Modeling more complicated molecules with beads is straightforward. In Figure 2, we show the bead valence sphere models for a few organic molecules including adamantane, cubane, and dodecahedrane. In these models, every bead again represents a valence electron pair. To prevent the beads representing electron pairs located at the end of a tree-like molecular graph from falling apart, we deliberately introduce small beads to hold these spherical beads together.

According to H. Bent, we can view the construction of Lewis's electron-dot structure of a molecule as the lowest-level molecular analog computation [7]. whereas the construction of a space-filling valence sphere model of a molecule corresponds to a higher-level molecular analog computation that gives approximate electron density profiles. Thus, using only strings and beads, we can construct a crude but shrewd electron density profile of a molecule without referring to Schrödinger equation. Making a beaded molecule is just like performing a molecular analog computation.

Using beads to model three-dimensional structures of fullerenes is easier than modeling molecules with tetravalent carbon atoms. In this case, the extra π electrons become delocalized over the molecular framework defined by the σ electron pairs. Their three-dimensional structures are determined mainly by interactions among the σ electron-pair domains. Surrounding every carbon atom, there are three electron pairs that could again be modeled approximately by spherical beads. Since there are no CH bonds in this



Figure 2: *Bead valence sphere models of adamantane ($C_{10}H_{16}$), cubane (C_8H_8), and dodecahedrane ($C_{20}H_{20}$).*

kind of molecular systems, the figure-eight stitch can easily be applied to create loops of carbon atoms sequentially.

Sierpiński buckyball

One unique feature of mathematical beading is that this method can be easily extended to larger molecular systems that contain several thousands of atoms. Building complicated molecular structures is no more difficult than simple structures such as C_{60} . As an illustration of the computational power of mathematical beading, here we show that the three-dimensional structure of a two-layer Sierpiński buckyball, or simply super buckyball, can be modeled realistically with this technique.

Super buckyball is a closed surface of genus 31 created by merging 60 buckyballs. In a sense, one can get this kind of structure by replacing each vertex in a truncated icosahedron with an artificial atom, i.e., a buckyball drilled with three holes at suitable positions, and each edge replaced by a short carbon nanotube. The general structural rules for creating super fullerenes through fusing small cage-like fullerenes will be described in another short paper for this Bridges meeting. In Figure 3 (left), we show the molecular structure for a particular super buckyball, C_{60} , denoted as $C_{60} \otimes C_{60}$ owing to its fractal nature. The bead model of this molecule is shown in the right of figure 3. In total, 6750 beads are used to mimic σ -type electron-pair domains in the molecule.

It is of interest to compare the structures of super buckyball to the high-genus fullerenes we described before [2]. In fact, superbuckyball is a high-genus fullerene of genus 31, which can be derived by subtracting one from the number of faces in a buckyball. The most important difference between these two types of high-genus fullerenes is the orientations of the necks, i.e., those regions with negative Gaussian curvature, relative the surface of the overall polyhedron. In the original high-genus fullerenes, the orientations of the negative necks are along the normal of the polyhedron. Here in the super buckyball, the orientations of the negative necks, created by fusing two neighboring C_{60} , are lying on the surface of polyhedron and along the directions of its edges.

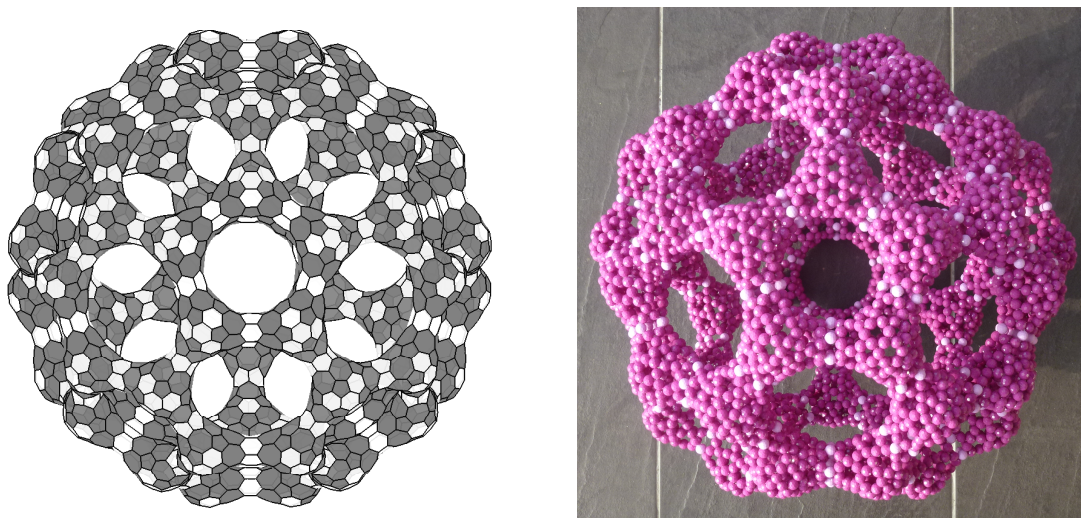


Figure 3 : *Bead model of superfullerene $C_{60} \otimes C_{60}$ with local C_3 rotational symmetry.*

Conclusion

We show that bead models can be viewed as the macroscopic realization of valence sphere models of chemical bonds. The repulsion among beads and the string that hold beads together can mimic the nature of chemical bond in fullerenes and many other molecules. The saturation and directional character of chemical affinity fall out naturally in bead models. We also point out that constructing a molecule with mathematical beading is actually a kind of analog computation. The result of the computation is the molecule's approximate three-dimensional structure.

We believe that not only can we model microscopic molecular structures with mathematical beading, we can also work in reverse to blur the boundary between chemistry and art so as to create new forms of bead sculptures that are inspired by the diversity and beauty found at the nanometer scale.

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