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Molecular Rendering with Medieval and Renaissance Color Theory

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Abstract—**This paper describes the application of Medieval and Renaissance color theory to the computer graphic rendering of molecular models. In particular, Alberti's and Cennini's color theories were employed to render shaded geometric primitives such as cylinders and spheres that are the components of traditional ball-and-stick and space filling molecular models. These results were compared with standard rendering based on the OpenGL API or through ray tracing. It is found that by implementing Alberti's and Cennini's color theories as color maps within a simple chemical illustration program it is possible to create molecular imagery comparable to contemporary computer graphics schemes.**

Keywords-molecular visualization; artist color models; art.

I. Introduction

"It must be recalled that a painting, before it is a war horse, a nude or some anecdote, is essentially a flat surface covered by color assembled in a certain order."
Maurice Denis

Geometry alone is not sufficient to provide the visual cues required for perception. In its abstract limit, geometry deals with an ideal world of dimensionless points, lines of infinitesimal diameter, and planes with infinite boundary. As cast within a computer visualization context, geometric representations are typically minimally expressed on a monitor or paper. By judicious application of color and texture to geometric representations it becomes possible to create more visually stimulating, natural looking scenes. This task is usually accomplished in computer graphics and visualization by rendering a scene employing linear perspective in concert with an optics-based lighting model.

The Renaissance development of linear perspective is well known. Fillippo Brunelleschi, an artist and architectural engineer (1377-1446), is attributed with the institution of visual perspective and the application of this optical theory to painting [1]. By placing the artist's/viewer's eye position at an image's center point and defining a horizon line he made it so all parallel receding edges of buildings appear to converge to a center point creating an illusion of depth. Art historians believe Brunelleschi's painter friend Masaccio explored these procedures in his work on the Trinity fresco in 1426, the first perspective demonstration directly influenced by Brunelleschi. Leon Battista Alberti, a lawyer, natural philosopher, artist, and architect, educated in Euclid's, Ptolemy's, and Alhazen's Optics as well as Euclid's geometry, endowed Brunelleschi's empirical methods with a firm mathematical underpinning. In his seminal treatise *On Painting* (*De Pictura*, 1435) he proclaimed Brunelleschi's work to be a scientific principle of art [2], and proceeded to recast it in the language of Medieval optics. Perspective then became a system for recording the intersections of light rays on a plane as they proceeded in a pyramidal pattern from object to eye.

Optics-based lighting is another matter. Geometric optical theory had existed at least from Hellenistic times (323 – 146 BC) [3]. But it was during the thirteenth century that optics became the premier medieval science and an integral component of the university curriculum. The teaching of optics was most influenced by the Islamic natural philosopher known as Alhazan who lived from the late tenth to early eleventh century. Alhazan revised and enhanced Greek optics by first recognizing that light was transmitted, reflected, and refracted into the eye, not out of the eye as theorized by the Greeks. He analyzed mathematically the nature of radiation associated with light and color, reflection and refraction, and even offered an influential discussion of the psychology of visual perception. Integral to his work was the direct experience of natural phenomena analyzed through mathematics.

While formal study and teaching of optical theory proceeded in parallel at medieval universities, the practice of painting by artisans essentially relied on a growing set of prescriptions or procedures for rendering spatial relationships and portraying light and shadow. By the onset of the fifteenth century artists had already become facile observers of nature, creating vivid images of flowers, animals and other objects, precisely recorded with characteristic features accurately detailed [4]. This artistic practice was codified in texts by thinkers and practitioners such as Leon Battista Alberti and Cennino Cennini [5], both of whom included the specification of systems for modeling color to render shadow and light.

These color models and those that followed influenced succeeding generations of painters. The Impressionist painters in the late 1800's relied on color modulating methods that were similar to the Cennini system. Auguste

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Renoir and Edgar Degas traveled to Italy and read Cennini's handbook. While other artists like Monet, Pissaro, and Cezanne began to work *plein air*, painting landscapes with a large number of pure hues, reviving the use of Medieval and Renaissance color models in creating brightly lit landscape paintings and figurative works with bold contrasting shadows.

By the turn of the twentieth century artists had begun to detach color from representation. In paintings by artists like Wassily Kandinsky, Mark Rothko, and Piet Mondrian color is not used as a modeling device to depict three dimensional surfaces, or to represent a landscape, still life or figure. Rather it is used in planes to divide the canvas, or as veils of color on the surface of the work. Color could symbolize, energize, or decorate the surface without regard to illusion.

Today, visualizers are as free as contemporary artists in their use of color. Because data and color may not be intrinsically related, color may be used in any fashion to craft an image that maximally communicates data's meaning. Yet, the beauty of art has stimulated the development of computer graphic rendering methods influenced by artistic styles and techniques. Non-photorealistic or expressive rendering has looked to art and illustration for its inspiration, generating a wide range of rendering methods from line drawings to water colors and oil paints [6] [7]. A number of visualization researchers have taken inspiration as well, either applying existing expressive rendering methods to visualizations or developing new ones [8] [9].

One area that remains open for research is the application of artist-created color models to visualization applications. And that is the focus of this paper. Specifically, Alberti's and Cennini's color theories are applied to the rendering of geometric primitives that are the basis for scientific visualization software. Our goal is to explore how well these artist color theories compare with standard optics-based lighting methods for rendering primitives such as spheres and cylinders. One application area in which visualization software relies heavily on these primitives is molecular visualization, where they are the foundation for creating the traditional ball-and-stick and space filling molecular models. Conceptually, molecular visualization makes a good comparative test case for artist theories because visualization and illustration have had a long history in chemistry, predating by a century the invention of computer graphics and visualization. And like the Medieval and Renaissance artists who experimented with the use of color, chemists have continually experimented with and invented new ways of visualizing complex chemical information. The seminal work of Cyrus Levinthal at MITs Project MAC in 1965 is an example [10]. It was one of the first applications of interactive computer visualization. In applying Alberti's and Cennini's color theories to molecular graphics we are continuing in the tradition of chemical visualization while benefiting from the rich culture of theory and experimentation that exploded in Italian Renaissance art.

In the following section we will briefly discuss methods used. Section 3 presents a discussion of painting and color. It will be followed by the application of Alberti's and Cennini's color theories to molecular display. Section 5 puts forth comparisons between contemporary rendering methods and molecular rendering employing artist models. The paper will conclude with a summary and discussion.

II. Methods

To generate a comparison between artist theories and contemporary visualizations of molecular models a three step process will be followed. First, an artist will paint an image of a ball-and-stick molecular model from observation of a traditional wooden model under room illumination employing the theories of Alberti and Cennini. Second, the theories of Alberti and Cennini will be incorporated into a molecular illustration program to render images similar to the paintings. And third, the molecular illustrations will be compared with the optics-based rendering methods that chemists use to generate their interactive visualizations and publication quality illustrations.

The artist color models were implemented in *Schakal,* a molecular illustration program designed to facilitate the creation of publication quality molecular rendering, typically line drawings [11]. Written in the 1980s, its raster images are rather minimal in comparison with contemporary molecular visualization standards. *Schakal* supports only a palette of 256 colors with smooth shading simulated by dither. Yet it can produce Phong-like shaded images of space-filling and ball-and-stick molecular models including cast shadows without formally invoking the Phong algorithmic form. Instead, it contains a simple empirical linear model that allows users to create and modify darkening functions which define the extent of an object's specular highlight and the rate at which the total illumination declines across its surface. This function is used to create a color table in *Schakal,* which is then sampled by employing the angle between the surface normal at a pixel and the light source vectors as an index to the color table. *Schakal's* strength for this research is its ability to allow a color map to be defined so that Cennini's and Alberti's color models may be transformed into color maps used for molecular rendering.

Schakal's images were compared with images created by Accelrys' Discovery Studio (DS) Visualizer [12], the Mercury Crystal Structure Visualization System from the Cambridge Crystallographic Data Centre [13], and the POVRAY raytracer [14]. DS Visualizer is a commercially available OpenGL-based molecular graphics program representative of a class of standard interactive molecular graphics systems [10]. The OpenGL API implements the Blinn-Phong lighting model with ambient, diffuse, and specular components and adds an emissive term [15]. DS Visualizer allows these terms to be adjusted to create shaded molecular models and has preset parameters that create the look of chalk, metal, and plastic. Mercury's capabilities are similar to DS Visualizer with extended ability to build crystal structures. The POVRAY raytracer can employ a wide range of illumination models, including radiosity, but for the comparisons here, it generated Phong-shaded geometric primitives with point light sources and material properties that are consistent with DS Visualizer. POVRAY was selected because of its availability and ability to render molecular graphic scenes. Many molecular visualization programs export POVRAY input files, as do the former two software packages.

III. Painting and Color

Painters create natural looking scenes by applying colors that vary in hue, saturation, and lightness (value). The colors available to painters form a relatively small palette of naturally occurring or synthesized inorganic and organic chemical compounds. The colors these substances exhibit are not only a function of their absorption spectra, but depend on crystal structure, particle size and shape, state of agglomeration, and presence of other materials. For example, cadmium yellow and cadmium orange are two pigments created with pure cadmium sulfide (CdS). The difference in color is created by a variation in the particle size of the solid. Finely ground CdS appears as a light yellow, while coarsely ground CdS is medium-orange. The color range of CdS may be extended by controlled substitution of selenium for sulfur. Selenium substitutes directly for sulfur into the cubic lattice, changing cadmium's coordination and hence, spectral environment. With appropriate proportions of S/Se it is possible to create an extended range of colors: orange, light red, bright red, dark red, maroon red and dark maroon [16].

In order for painters to create complex images with subtle hue differences they must mix paint or pigments. To rationalize the process they use a color space based on the primaries red, yellow, and blue arranged at the corners of a triangle. Secondary colors are created by equal mixing of adjacent primaries. For example, yellow plus blue makes green, red plus blue makes violet, and red plus yellow makes orange. These six colors form the traditional color wheel and spectral sequence: red, orange, yellow, green, blue, violet.

A painter's color wheel begins with this sequence and adds six additional hues by mixing: orange-red, orange-yellow, yellow-green, blue-green, violet-blue, and red-violet. These hues are arranged in the wheel to express color relationships, but not absolute truths. For example, opposite hues on the wheel are complementary colors. Green is opposite red, meaning red is pure, totally devoid of green color. However, as we have noted, many pigments and paints begin as spectral or chemical mixtures making them *impure* colors. This makes color mixing a more complex task. In theory, yellow and blue combine to make green. But with paint, some yellows are better for making green and others are better for making purple. Pthalocyanine (pthalo) blue and lemon yellow can be combined to make an intense green. An artist may also use cadmium yellow, a yellow with a hint of red, and pthalo blue to make a more muted green. As a result an artist will usually have at least two different reds, blues, and yellows. All of those colors have the possibility of being combined with each other.

Mixing paints, even colors like pthalo blue and lemon yellow, mutes the intensity or purity of each color. For a more intense green a painter could use viridian green straight from the tube. For variety, an artist might mix viridian with lemon yellow or with pthalo blue. Each time a paint color is mixed with another paint color the intensity or purity of the color is reduced. Therefore some painters resort to using as many pure pigments as possible. Paul Cezanne used a palette with up to thirteen different colors, plus white. This larger palette of colors allowed him to apply more colors purely from the tube without reducing the intensity of the relatively pure pigments [17].

In addition to hue, its purity, and the relationship between different hues, there is also the value of a hue. Value is a means of measuring a hue's lightness or darkness. Yellow has a high key or light value; blue has a low key or dark value. White can be added to a color to increase its value. Ultramarine blue is a very dark blue with reddish qualities. When white is added to ultramarine it is increased in value and will actually appear to become bluer. As the amount of white is added the color will eventually become very light, chalky looking, until its original color is impossible to discern. The addition of white to pure colors creates tints. Adding black to hues has the effect of decreasing their values, producing what is known as shades.

Artists frequently manipulate closely valued tones by using colors to create warm or cool darks and lights. This is a relative process. Although a pure red is generally thought of as warm and a pure blue, cool, other colors like yellow, green, and purple vary depending on the component colors used to make those colors. While color on its own may be warm or cool, colors are usually judged in relation to each other. A yellow might be warm in relationship to gray and cool in relationship to some reds. Warmer colors usually appear to advance toward the viewer, while cool colors recede from view. Hence, painters will use increased amounts of blue to indicate distance in a painting to create atmospheric perspective.

In sum, the diversity of techniques developed to create paintings was communicated by practitioners and scholars in treatises that codified these methods by the beginning of the fifteenth century. Such treatises were used for both educating artists and creating theoretical foundations of artistic practice. In the following section we will address two such methods and employ them in the computer rendering of molecular illustrations.

IV. Color Systems

In 1390 Cennino Cennini composed *The Craftsman's Handbook*, one of the earliest compendia of artists' methods [5]. One section of his text describes the painting of drapery. Well trained artists were expected to be able to simulate the bending and folding of cloth as it draped over tables, chairs, and of course, on and over people as clothing. Cennini attempted to systematize the procedure by recommending a series of steps, beginning with the creation of colors to be used. He recommended taking three bowls and mixing a tiny bit of white with the pure color in the first bowl. The second bowl should contain a large amount of white with the pure color. The third bowl would combine an equal mixture of the first two bowls, resulting in a medium tint. He suggested that the artist use the color with the least amount of white to paint the folds of the drapery that were darkest. Then paint in the intermediate tone for the upper layers of the folds of drapery, saving the lightest tint for the topmost part of the folds. He suggested using pure white for the portions of drapery most intensely lit. Cennini prescribed pure color for the part of the form in greatest shadow. By this simple blending of tints Cennini created a color map where white is used for rendering the brightest surface highlights that directly face the light source, to blends of color and white for medium brightness regions, to pure color for surfaces that are obscured from the light source.

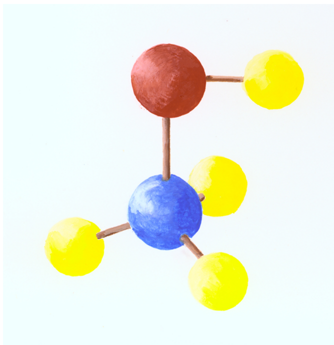

Figure 1. Artist rendering of methanol molecule using Cennini's color model

Cennini's three bowl color mixing rule has been applied to two watercolor renderings of the methanol molecule (Figs. 1 and 2). The artist painted directly from a traditional wooden ball-and-stick model illuminated with natural northern light from the upper left portion of the frame. In the first image (Fig. 1) the original color scheme is replicated: yellow for hydrogen, red for oxygen, and light blue for carbon. In the left-hand image of Fig. 2 the color scheme has changed to blue for hydrogen, red for oxygen, and green for carbon. This change was made because yellow is a problem. Bright yellow rendered against a white background provides little luminance contrast, thereby making it difficult to see the yellow spheres against the white background. By replacing yellow with ultramarine blue the luminance contrast between sphere and background is maximized.

The right-hand image of Fig. 2 shows the result of adapting Cennini's three bowl method to the color maps in the *Schakal* molecular rendering program. In both watercolor and computer graphics the edges of all forms contrast sharply with the pale background enhancing viewability. In particular, the ultramarine blue, used in a nearly pure color, looks appropriately dark in the self-shadowed regions of the spheres lying distal to the light source. This works as well for the green hue, but red is problematic. The contrast between light and dark areas for the red sphere is less than that for blue or green. Contrast between shadowed and highlighted areas of spheres may be enhanced by blending in more white but at the cost of dilution of the red hue. The situation the painter is faced with here is similar to the one found in a Fra Angelico painting.

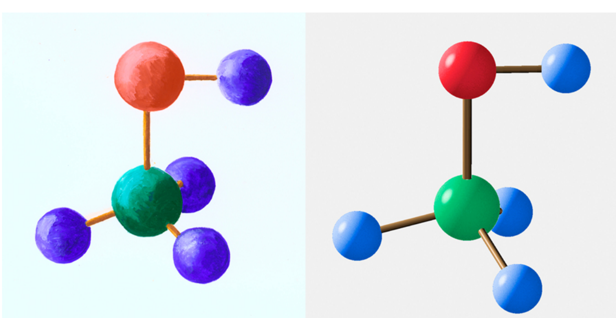

Figure 2. Artist rendering of methanol molecule (left) and computer image (right) using Cennini's color model

The Annunciation by Fra Angelico is a painting of a New Testament text where God sends an angel to announce to Mary that she will bear a child named Jesus, who is the Son of God (Fig. 3). Fra Angelico uses Cennini's three bowl method to paint Mary's and the angel's red robes. The angel's drapery is red and gold, modulated with white tints of the colors in the highlights and pure color in the folds. It appears that the red used on the angel is mixed with more white than that coloring Mary's robe. The gold stripes are close in value to the red stripes, and the gold tends to blend in with the surrounding color of the portico. The angel's clothing causes it to meld with the predominantly gold portico.

Figure 3. The Annunciation by Fra Angelico, Cortona, 1433 -1434.

In contrast, Mary's dark drapery isolates her from the surrounding colors. Mary's red robe thrusts out from her surrounding blue drapery, the folds of Mary's blue drapery have more depth than the folds of her red robe. This is because darker tones of blue recede from the viewer more than pure tones of red. Fra Angelico used the colors to create a colored jewel, with Mary and her red robe highlighted within the dark surrounding of the blue drapery lined with black. His method of using pure tones for shadows does not create deep shadows. Instead, color is used to isolate Mary from the surrounding scene. These pure colors create a richness that was prized in the early fifteenth century.

Cennini described another method for modeling color. This method was used by many artists, including

Michelangelo, who employed this technique on parts of the Sistine Chapel ceiling. The method involved using various hues to model drapery instead of using the three bowl method of pure hues modified by white. For example, in a drapery of gray, Cennini prescribed using white or yellow for highlighted areas. Violet, black, or dark green were suggested for shadowed areas of gray drapery. One important aspect of this scheme of modeling is that it relies upon colors of lighter value than the main color for the highlights, while colors darker than the main color are suggested for the shadows. Table 1 shows some of the color relationships that were suggested by Cennini.

TABLE I. CENNINI'S COLOR RELATIONSHIPS

Main Color	Lights	Shadows
Gray	Yellow or White	Violet or Black or Dark Green
Red Purple	Pink Flesh or Yellow	Pure Red Purple or Violet
Ocher (dull yellow)	White or Green	Black with either Sinoper or Hematite (brown reds)

Fig. 4 is an example of a methanol molecule modeled using this method. Each atom of the molecule is modeled using three colors: the main color, the highlight color and the shadow color. For the hydrogen atoms, the main color is gray with yellow and violet used to indicate highlights and shadows. The violet color being darker than the gray provides convincing shadows. Also the violet color blends more easily with the gray providing a smooth transition from gray to violet. The yellow highlights are more discordant in relationship to the gray and tend to look more like specular highlights rather than merely lit areas. Using blue in the shadows or violet on a gray, blue or red shape is a harmonious way to indicate shadows. Blue is a better way to indicate shadows than using pure red on a red molecule for shadows. These atoms do have a rich appearance. If the colors are blended sensitively than the effect is one of liveliness. On the other hand, if this method is used too broadly or crudely it results in chaos and discordance that detracts from the goal of modeling lights and shadows.

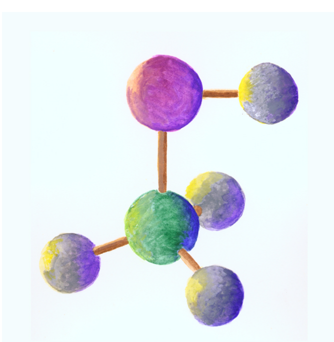

Figure 4. Cennini's alternative color model applied to artist's rendering of methanol.

Artists in the time of the Renaissance used this method to model angels or parts of paintings. Michelangelo used this method to model the drapery of the sibyls and seers contained within the spandrels and lunettes of the Sistine Chapel ceiling. Raphael used this method to depict people bathed by the light of heaven, while he reserved less highly colored methods for modeling other parts of a painting.

Another compendium, *On Painting,* was written by Leon Battista Alberti in 1435 [2]. In it he stated that white and black are at the extremes of light. The artist should use black to indicate the absence of light and white to indicate the brightest light. Fig. 5 shows the methanol molecule modeled using Alberti's suggestion. It is easier to achieve a good three-dimensional model using black and white for modeling than using either of the methods suggested by Cennini. Using pure hues for shadows means that in many instances there is no capability for creating a dark value. When the hues are varied, for example using yellow to indicate light on a gray object, then it is difficult to maintain a unified sense of form. But using black and white to modulate a color is in keeping with our eyes' ability to best determine form in black and white. Given this and the fact that his observations concerning light's interaction with matter are consistent with optics-based illumination models, Alberti's theory will be used in the following comparisons of visualizations generated by three programs.

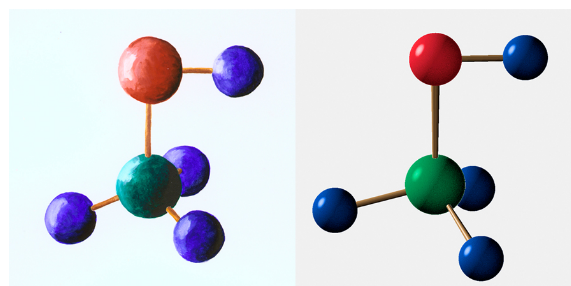

Figure 5. Artist rendering of methanol molecule (left) and computer image (right) using Alberti's color model.

V. COMPARISONS

Three images were created to compare the color map representing Alberti's color theory with the three contemporary rendering programs specified in Section 2. Alberti's color map expressed within *Schakal* begins with white for highlights, blends with an increasing percentage of hue until a pure hue is attained, and then blends hue with black until 100% black is reached (c.f. Fig. 5).

Fig. 6 shows a space-filling model of a crown ether molecule drawn by *Schakal* employing Alberti's color map (left) adjacent to the same molecule rendered using OpenGL by DS Visualizer (right). A single point light source illuminates the models from the upper left. Overall, both *Schakal* and DS Visualizer create comparable images. The greatest variance comes in the differences found in the size and color of specular highlights. With some work it would have been possible to make these highlights coincide, but the similarities in overall shading are sufficient to demonstrate the close approximation Alberti's model makes to the OpenGL rendering.

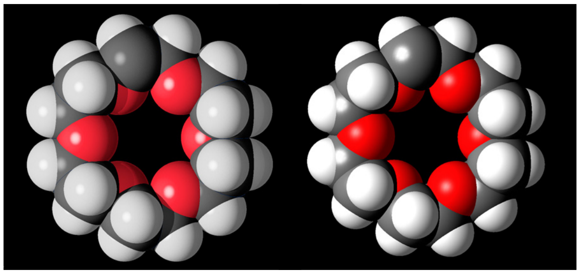

Figure 6. Schakal (left) and DS Visualizer (right) space-filling renderings of crown ether molecule.

Fig. 7 displays a ball-and-stick model of the caffeine molecule rendered by *Schakal* (left) and POVRAY (right). As with Fig. 6, *Schakal* and the raytraced image and are in accord. The major difference between these images resides in *Schakal*'s darkening function. Here the caffeine molecule rendered by *Schakal* appears as if it is nearer to the light source than that created by POVRAY. However, the shapes the cylinders and spheres are well represented by Alberti's model.

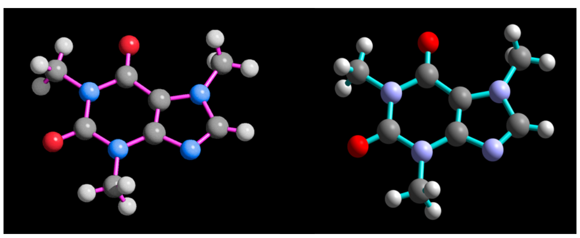

Figure 7. Schakal (left) and POVRAY (right) ball-and-stick renderings of caffeine molecule.

A view of the cubic zirconium crystal lattice rendered by *Schakal* (left) and Mercury (right) is shown in Fig. 8. In contrast to the previous two images, the flatness of the visual field has been replaced by an enhanced depth accentuated through a single point perspective projection. Both images were created from comparable viewpoints, but Mercury's OpenGL rendering presents a slightly larger angle of view than that rendered by *Schakal*, thus increasing the images sense of depth. Mercury's control over OpenGL's lighting model is less flexible than DS Visualizer's, reducing the viewer's ability to manipulate the oxygen atoms' (red spheres) highlights so as to make them comparable to *Schakal's.* Despite these differences, Alberti's illumination model generates a comparable image to OpenGL's.

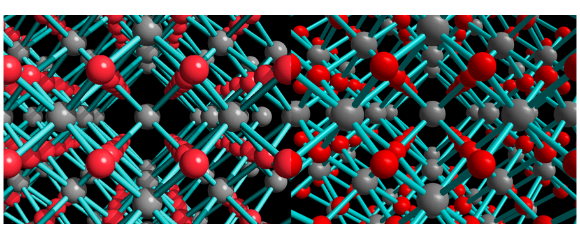

Figure 8.Schakal (left) and Mercury (right) ball-and-stick

VI. Discussion

We have considered the application of Medieval and Renaissance color theory to the computer graphic rendering of molecular models. In particular, Alberti's and Cennini's color theories were employed to render shaded geometric primitives such as cylinders and spheres that are the components of traditional ball-and-stick, and space filling molecular models. The three comparisons given in Section 5 demonstrate that Alberti's paint model, implemented as a color map, can generate visualization imagery comparable to the optics-based Phong shading model for these fundamental geometric primitives. What we have done here is to automate the perceptual process so that the painter's practice of determining a light source's orientation relative to a surface in a scene is transformed into a computation of the angle between a surface normal and the light source vectors; and the artist's color selection is converted into a color look-up from a table. In so doing we have made a connection between the artist's empirical model of illumination and the perception-based illumination model of computer graphics that is founded on geometric optics [17]. The fact that this translation can be accomplished so easily and that it produces images of comparable quality to the formal theory is a validation of these Medieval and Renaissance methods.

We have also compared Alberti's and the Cennini's color systems as they relate to the rendering of molecular structure. In general, both methods deal with the three properties of color - hue, value, and saturation. Each focuses on the modeling of value. For Cennini, only one way exists for changing value, which is the addition of white to the pure color. For Alberti there are two – value is increased by adding white and decreased by adding black, so as to create a complete range of colors with white highlights as needed. As such, Alberti's model creates an image consistent with optics-based methods for rendering of the effects of illumination. Yet, Cennini's shading method does provide sufficient visual cues for perception of structural attributes of surfaces as is clearly seen in Fra Angelico's painting (Fig. 3), and in both the artist and *Schakal* rendering of methanol (Fig. 2). The strength of Cennini's method is that it relies heavily on the use of pure saturated colors to create imagery that possess an eye-popping vibrancy. This effect, as we have noted above, was not lost on the Impressionist painters who employed it to transform the way we view light and color in paintings. This is a point worth further investigation.

Finally, much of our discussion has focused on a painter's selection and use of colors in concert or in opposition to create images that exhibit a coherent integration of parts. Color selection and integration into an artwork is part of an artist's training, and is an important component of how any color model is implemented (see again the discussion of Fig. 1 as an example). Thus, regardless of the color theory employed, a competent visualization must be made with color selection as a primary consideration.

Acknowledgment

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