Molecular Art In Evolution

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Evolution on various levels provides analogies between sciences and art

Abstract

The evolution of an actual chemical reaction between molecules, a process often giving the experience of artful shapes and movements if modelled properly on a computer, does show many, deeply analogous features and processes with the actual history of various aspects of the evolution of life on Earth, as well as the evolution of human thought processes involved in Art, and especially, in Science-related Generative Art.

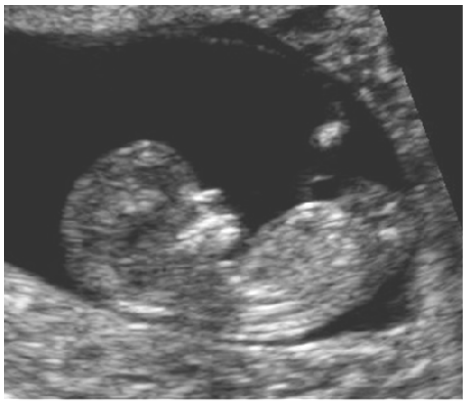
Many of the fundamental components of the changes in Nature and the changes in our perceptions of artful forms, that are accessible today even on the sub-microscopic level of individual molecules, are following highly similar changing patterns and modifications, just as the initial impression of looking at an artistic painting is also evolving, leading to sequences of associations and interpretations, developing, maturing, and becoming a better match, in some sense, more fit, as they enter, and make room for themselves in the collections of our artistic and scientific experiences.

In this contribution, several examples are shown, aimed at enhancing the strong connections among various levels of evolution, in Nature, and in our minds.

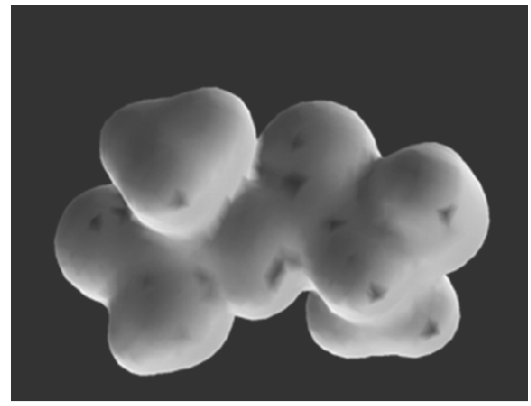
1. Evolution in Nature, Evolution of Individual, Molecular Evolution, and Evolution of Ideas

Evolution in nature, with all of its complexity, shows many analogies to fundamental processes on very different levels, for example, to the evolution of an individual, unborn human being to an active, thinking individual capable of appreciating both science and art, including their intriguing combination: Generative Art. These analogies are also strongly manifested in the actual, physical level of molecular processes, leading to intriguing shapes of artistically appreciable molecular forms, and also on a far more abstract level of evolution of ideas within the domain of human culture.

Figures. Evolution of an individual human in time, and the "abstract" evolution of Molecular Model as accurate low electron density becomes accessible



Evolving Individual



D-alanyl-D-alanine Molecule

Evolution is usually considered as a process in time, however, in a more general sense, evolution can be considered to represent changes along some coordinates different from time. For example, in the case of molecules, the evolution of our growing understanding of their behaviour, clearly a time-dependent process, correlates with another coordinate: it has become possible to model reasonably accurately the low electron density cloud outer regions of molecules only recently, due to the actual evolution of advanced quantum chemistry computer modelling methods. Hence, some sense of evolutionary change can be associated with the gradually diminishing density of electronic cloud as we consider molecular shapes further and further away from the atomic nuclei present in the molecules. In this sense, the value "ro" of electronic density, that happens to be 0.01 atomic unit, is also a coordinate for some type of evolution on the right side of *Figure 1,* a figure showing not only an evolving human on the left hand side, where evolution is, indeed, considered along the usual time coordinate, but also the dipeptide D-alanyl-D-alanine, where the electron density parameter "ro" is some "abstract" evolutionary coordinate, only analogous to time, the time-coordinate, that in turn is the most relevant to the evolution of the unborn individual on the left hand side of the figure.

2. How molecules, their shapes, and interactions show analogies with aspects of evolution

The direction of changes in all types of evolutions is influenced by a multitude of factors, however, some factors are often dominant, related to the physical concepts of energy and entropy. Processes left to their own without external influences often, but not always, progress from instable arrangements towards some more stable ones, and

also, time often tends to lead from well-organized arrangements towards toward some more disorganized ones. These factors can be considered as somewhat analogous with feasibility and probability, respectively.

In this context, if one considers the evolution of molecular interactions, which today can already be modelled rather reliably by quantum chemistry computational methods, often resulting in intriguing shape changes of the participating molecules, then the potential role of additional molecular parts as "helpers" in the process of evolving interactions provide new and intriguing features, worthy of the attention of Generative Art observers. In the following images two such scenarios are shown. In the first image, the "abstract evolution" of gradual refinement of the observed electron density values, from the "crude" 0.1 atomic unit (a.u.) value to the more delicate 0.001 a.u. value is shown, where the evolution is relevant to the interaction between a dimethyl-ether and an ethene molecule.

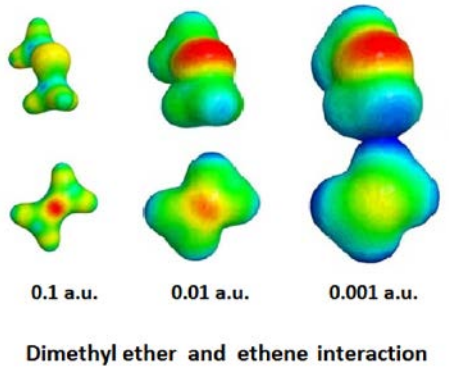


Figure 2. Evolution of molecular interactions between dimethyl ether and the ethene molecules as our focus evolves from the crude, high electron density value of 0.1 a.u. (atomic unit for electron density) to the fine, low density value of 0.001 a.u.

In the next image, in *Figure 3,* the same two molecular parts are considered, but with an intermediate molecular part added, essentially forming a benzene ring, that allows the local electron densities to interact more directly, "through chemical bonds", that is modifying the interaction process considerably. In reality, this "through-bond" interaction is the dominant, not surprisingly, after all, chemical bonds can be rather strong, keeping some molecules stable even at very high temperatures.

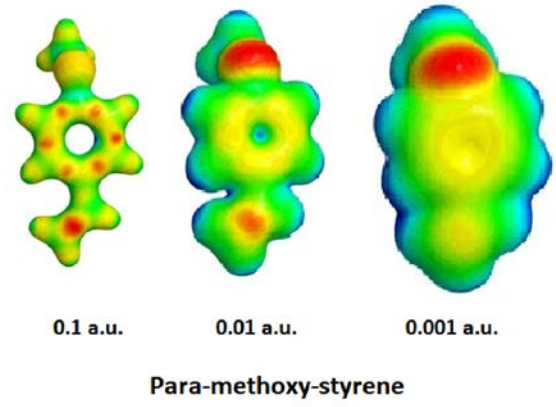


Figure 3. Evolution of "through-bond" type molecular interactions between dimethyl ether and the ethene molecules, as delivered by an intermediate molecular part, actually generating a benzene-ring structure, as our focus, again, evolves

from the crude, high electron density value of 0.1 a.u. (atomic unit for electron density) to the fine, low density value of 0.001 a.u.

Nevertheless, both sets of images provide an interesting glimpse into the "interaction-evolution" world of some molecules, which are, in some respect, representing some typical processes which often occur on the micro-microscopic level of the molecular world. In both of these images, the colour changes represent the changes in the so-called "electrostatic potential", a descriptor providing an indication, how some, hypothetical "wondering local charge" "would like" to be present at the given location, with red colour indicating the strongest such interaction. Whereas in practice no such wondering point charges can be moved along such surfaces, nevertheless, this "artificial experiment" provides chemically useful predictions for the likely locations, where a given molecule would prefer to initiate a reaction with a suitable partner molecule. It is a sombering thought to remember, that in every millisecond of our lives, more than million times million such reactions occur in our bodies, providing the very foundations of life. Hence, the study of molecular shapes and shape variations (see, for example, references [1-8]) are having connections to many fields beyond chemistry, involving biology, pharmacology, medicine, and in a broader sense, very few industry may claim to have no direct use of at least some of the benefits the information on molecules can provide.

Some of the original investigations leading to these images have been addressing the more general problem, how interactions develop and spread through various regions of molecules ([4],[5],[6]). Some of the fundamental relations are discussed in references [7] and [8], however, the original studies first using "missing molecular parts" for the analysis of interactions evolving exclusively through space or using in addition a through bond mechanism, have been described in references [9], [10], [11], and [12].

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