

Philosophy of Computational Chemistry: On the Way to an Interdisciplinary Epistemology?

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Biological Systems have provided much of the inspiration for the development of supramolecular chemistry. As a consequence, many synthetic supramolecular systems have been designed to mimic the structure or function of more complex biological processes. Actually these models (artificial, abiotic or non-biological molecules) are designed by working groups connected with computational chemistry, a field of knowledge in which interdisciplinarity lies at the basis of all their molecular architecture. We are therefore face to face with a different approach to chemical phenomena, in which the application of systemic Paradigm assumes a very special emphasis mainly in the case of computational chemistry based on simulation a third type of scientific knowledge. We are dealing with a different way of thinking science with awareness that scientific world vision is a continuously changing flow in which uncertainty and complexity are seen as useful tools for interdisciplinarity. The philosophical interest of this approach is connected with two different ways of looking at chemistry, especially in the case of computational chemistry:

The Epistemological Approach – because it deals with language and classification in chemistry and biochemistry.

The Ontological Approach – because it is concerned with concepts related to the philosophy of chemical reactions or philosophy of matter, inasmuch as matter is made up of chemical bondings.

Science became epistemic, once the theories say more about the minds that conceived them rather than about the reality processes itself, because every theory is just an approach to explaining reality. On the other hand, reality is a process of information exchange among all living beings at their own different levels (Biological, Physical, Psychological and Social).

We are developing a scientific model based on the concept of relationship or interaction – a much broader concept than the analytical one which is still used by “normal” science.

While mechanicism presents the world as an enormous deterministic machine, holism accepts all those “mechanic” characteristics but goes beyond them to see Nature as a much wider universe made up of a fantastic matrix of dynamic and organic interrelationships.

References

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Maria Burguete got her Ph.D. in History of Science (contemporary chemistry) from Ludwig Maximilians University at Munich, Germany (2000). She was the very first biochemist to graduate from the Faculty of Sciences in Lisbon (1982), after completing a Bachelor’s Degree in Chemical Engineering (1979) at the Lisbon Higher Institute of Engineering (ISEL). She is a scientist and a university lecturer with teaching & research experience in a wide variety of scientific fields. This diversity enhanced the development of both her interdisciplinarity and a transdisciplinarity. She is now a scientific researcher at Coimbra University’s Department of Computational Physics in Portugal. She has published five books in the scientific field (and five books of poetry) and over 20 scientific papers.