

Dimensional reduction in inorganic systems: From dissipative dynamics to artificial life.

Lee Cronin, Department of Chemistry, University of Glasgow, Glasgow, G12 8QQ, UK
Email:L.Cronin@chem.gla.ac.uk

Understanding supramolecular chemistry has allowed a fundamental change in the way chemists both perceive and investigate the chemical world. This because the process of molecular recognition, fundamental to the biological world (c.f. Emil Fischer - lock-and-key principle), was found to be vital in the chemical world. Manipulation of recognition along with the kinetics by which the process occurred also allowed the idea of 'self-assembly' to be conceived whereby well defined building blocks can be observed to assemble to complex and often highly symmetrical architectures. Although the concepts underpinning supramolecular chemistry are extremely powerful, the ability to produce highly functional molecular systems using a 'designed' approach seems to be extremely limiting. We are interested in using the principles of molecular recognition and self assembly under non-equilibrium conditions such that entropy is being 'exported' through the system - i.e. the system is dissipative. The idea is to allow the 'emergence' of new molecular organizations that may not be stable under equilibrium conditions and to utilize such systems to create highly complex functional architectures (c.f. the architectures present in a living cell).

In this respect there appears to be a fundamental gap in our understanding of emergent systems on the chemical level since although we all know what a cell looks like, understanding the cooperative dynamics that allows whole cell processes to function is far from reach. Also, the process of self assembly and organization of the components required for the emergence of life as we know it today is also far from being understood. I will start to argue that modeling (in chemical space and *in silico*) cooperative self assembly of dissipative systems is the fundamental key to development of non equilibrium structures that have well defined functions and information processing potential. I will also discuss our recent attempts to develop approaches for the experimental simulation of the assembly of artificial chemical cells (CHELLS) as well as a theoretical framework based upon a 'Turing' test for artificial life.[1]

[1] See: "The imitation game—a computational chemical approach to recognizing life"

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