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MULTISCALE SIMULATION: REDUCTIONISM OR EMERGENCE?

In his famous *Discourse on Method*, Descartes wrote: "The second precept is to divide each of the difficulties ... in as many parts as possible, and would be required to resolve the best." In another context, and many centuries before him, Aristotle stated that: "The whole is more than the sum of its parts." Nearly 2000 years apart, two very different conceptions of science, reductionism and emergence, confront. What implications these two views have in the scientific formalism of chemistry? Could this have an impact on the very future of chemistry? Indeed, the focus in reductionism has generally been the main development vehicle of chemistry, but the actual precept of emergence should also be associated with it. Indeed, how can we explain the functionality or the self-assembly of materials, the tertiary structure of proteins, the phase diagram, nanoparticles, crystallinity, and others, from the only knowledge of the structure of the molecule. One way to respond is to indicate that the complexity tends to grow. Then it is perfectly appropriate to specify that computers - more specifically multi-scale simulations - are becoming the tool of choice for stimulating answers. In this presentation, both concepts of reductionism and emergence, are exposed. They actually underline the difficult concept of the transition from the molecule to the macroscopic properties. For that purpose, two examples from the lab are discussed. The reductionism perspective is envisioned through the design of a new proton-exchange membrane for fuel cells applications. The emergence is anticipated by the simulation of the glass transition in polymers, and its chemist perspective.

Armand Soldera is currently a professor at the Université de Sherbrooke (Quebec, Canada), and vice-dean partnerships of the Faculty of sciences. He has been head of the department of chemistry (2010-2016), director of the Quebec Centre for Functional Materials (2015-2018). He received a Ph.D. in Molecular Physical Chemistry for his work on liquid crystals from the Université de Strasbourg in France. He was a postdoctoral fellow, first at the Université Laval in Québec, Canada, working in polymer and liquid crystal science, and at RUG in Groningen, Netherlands working on scattering of polymers. In 1994, he was hired by the French Commissariat à l'Énergie Atomique (CEA) as a research engineer in the military division, where he began to work on molecular simulations of polymers. He joined the Université de Sherbrooke in 2002 as an assistant professor in the chemistry department, became associate professor in 2005, full professor in 2009, and department chair from 2010 to 2016. He was adjunct professor at ISMANS (Le Mans, F.) since 1996. His research focusses on the study of the intimate link between micro and macroscopic scales in soft matter (polymers, liquid crystals, and organic glasses). To help him in this complex task, he merges together simulations and experiments following a multi-scale approach. With Prof. Theo van de Ven, he edited a book entitled Advanced Materials that will be published by De Gruyter in 2019.