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NANOMATERIALS: IN BETWEEN TRADITIONAL CONCEPTS OF UNDERSTANDING MATTER

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We classify macroscopic amounts of matter according to various concepts, as metals, semiconductors, insulators, atoms, molecules, complexes, polymers, and so on. Each of these terms triggers a specific image that has a consistent meaning throughout the scientific community. But which of these describe adequately an isolated nanocluster like Pt13? We use Newtonian mechanics to describe the frictionless, periodic motion of a system consisting of a few particles, and we can give trajectories and the momentum of every particle at each instant of time. In contrast, systems consisting of large numbers of particles are treated thermodynamically as ensembles in which the information of individual particles is lost and available only as a statistical average. Spontaneous processes occur under heat dissipation, are not normally periodic and approach an equilibrium characterized by a minimum in free energy. Is Newtonian mechanics or thermodynamics more appropriate for treating nanoclusters? Many of the concepts that we use to describe macroscopic amounts of matter break down for nanomaterials. Metals turn into semiconductors and insulators; phase transition temperatures shift dramatically, and the transitions broaden and disappear completely so that the Gibbs phase rule loses its meaning. Heat and temperature that are normally understood to represent kinetic energy are no longer well defined. According to traditional definition we may find that a small system cools down instead of heating up when we deposit more energy on it, pretending a negative heat capacity. Small systems are getting increasingly relevant in chemistry and physics, e.g. in catalysis, molecular electronics or energy devices. It is here where one starts to find amazing and perhaps disturbing phenomena, and these are becoming a hot field of research. Even in an expected thermodynamic system one may find quantum phenomena. The question comes up how we manage the transition between unexpectedly incompatible descriptions.

Biography

Emil Roduner studied Chemistry at the University of Zürich and at the Rensselaer Polytechnic Institute in Troy, NY. In 1988, he was awarded the Werner Prize by the Swiss Chemical Society for developing muon spin resonance to a universal method for studying structure and reaction behaviour of free radicals. During 1995-2012 he held a Chair of Physical Chemistry at the University of Stuttgart. After retirement he accepted a part-time Professorship at the University of Pretoria in South Africa. He wrote an advanced textbook, *"Nanoscopic Materials: Size-Dependent Phenomena and Growth Principles"* (RSC, 2014). His research interests include studies on structure, size-effects and magnetism of platinum nano-clusters and dynamics of molecules in the pores of zeolites, mechanisms of elementary steps in catalysis, kinetic isotope effects, degradation and proton conductivity of fuel cell polymer membranes. In South Africa, he is working on the electrochemical conversion of CO2 to liquid fuels using solar energy.

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