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Size effects in chemistry & physics of atomic & molecular clusters, nanoparticles & nanostructures

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"Small is different" – when particles reach the size of nanometers or below, material properties can become extremely size-dependent, often even sensitive to the exact number of atoms or molecules in the particle or device. This is a consequence of emerging quantum size effects, but also of structural changes compared to the bulk: when matter shrinks to nano-size or even below, its (relative) surface strongly increases and a discrete electronic structure emerges. The decreasing atomic (or molecular) coordination can even lead to the appearance of entirely new structural arrangements. This naturally affects the chemical and physical properties at the nano-scale, such as the geometric and electronic structure, thermodynamics, spectroscopy, dynamics, catalysis, magnetism, superconductivity, and optical properties, and finds applications in, *e.g.*, 2D materials, nanodiamonds, biotechnology, medicine, energy-related materials, catalysts, environmental science and astrochemistry.

Recognized by pioneers such as Jean Farges, Jacques Friedel, Walter Knight, Ryogo Kubo, and Bernhard Mühlschlegel in the 1970s, this led to the establishment of the conference series "**International Symposium on Small Particles and Inorganic Clusters – ISSPIC**" that since has continued to provide a vivid interdisciplinary platform to discuss this wide field of size-effects of atomic and molecular clusters, nanoparticles, nanocrystals, and nanodroplets. After the forced pandemic break, the 21st conference in the series, **ISSPIC XXI**, taking place from 3rd to 8th September 2023 in Berlin (Germany), aimed to reflect the current status of research in the physics and chemistry of small particles and clusters and to highlight new results, emerging trends, and perspectives. The present themed collection has been prepared on the occasion of ISSPIC XXI in lieu of a classical conference proceeding to address a wider circle of contributors.

The collection includes studies from theory and experiment, whilst in many cases a distinction is not meaningful as both have entered into a fruitful relationship. Typically, but not exclusively, this would be the case in the interpretation of spectroscopic data. Spectroscopy, making use of the wide spectral range from microwaves, over the infrared, visible and ultraviolet, to X-rays, has been and still is indispensable for the characterization of clusters, nanoparticles or nanostructures. The articles in this collection comprise a number of examples for such analyses of geometric, electronic and/or magnetic structures, and their changes with size.

Studies on isolated small clusters allow for a precise characterization of the size, composition, and chemical as well as structural properties, and thereby represent indispensable model systems for gaining a fundamental understanding of their size-dependent evolution. For clusters or nanoparticles deposited on a substrate, the interactions become more complex and the combined system may be overall structurally less defined (and more variable), but it can be much closer to real-world applications, like nanodispersed metal catalysts and electronic or optical nanodevices. Nanoparticles in electrochemical environments are even more intricate (**https://doi.org/10.1039/D4CP00889H**). Merging different cluster types, *e.g.*, metal clusters and fullerenes (or oxide clusters), leads to interesting intermediate systems that can be still small enough to permit gas-phase studies and the application of high-level theoretical methods, but already comprise some of the complexity related to the interaction with the support (**https://doi.org/10.1039/D4CP01398K**).

An important aspect of this themed collection is the size dependence of the particles' reactivity. In particular for gas-phase or surface-deposited particles, mass spectrometric techniques have been effective for the identification of highly reactive clusters as well as the detection of reaction products and allow for studies of reaction kinetics and thermodynamics (**https://doi.org/10.1039/D3CP05862J**). Thereby, fundamental insights into the relations between

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electronic and/or geometric structures and reactivity have been gained. Several contributions to this collection demonstrate the great potential that infrared action spectroscopy has for understanding small-molecule activation by metal or metal oxide centers, reactions that are central for many catalytic processes (**https://doi.org/10.1039/D3CP04035F**).

Besides the size of a particle, naturally also its composition has an effect of its properties. This gives an additional parameter for selective control of chemical and physical properties. Several contributions to the collection demonstrate how the controlled addition of single or few dopant atoms (or molecules) can have a pronounced effect. The dopant may just be introduced for a more subtle modification of the underlying electronic structure to steer reactivity (**https://doi.org/10.1039/D4CP00857J**) or optical properties. In other cases, completely new characteristics can emerge, like is seen, *e.g.*, for the magnetism of – initially paramagnetic – tin clusters when they get doped by single transition metal ions (**https://doi.org/10.1039/D4CP00890A**). When the fraction of dopant atoms is strongly increased, like in nanoalloys, segregation and ordering effects can occur that depend on cluster size and shape (**https://doi.org/10.1039/D4CP00979G**).

The collection presents a comprehensive view of the current topics in cluster and nanoparticle research. It gives a broad overview on the spectrum of methods that are used to characterize them, both by experiment and theory. The contributions demonstrate the diversity of the scientific approaches, with one central motivation being the quest for a fundamental understanding of the emergence of properties in the nano-regime, but also targeting applications, *e.g.*, through an enhancement of particle stability or a better control of substrate interactions.

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