Preface

Atomic clusters are aggregates of atoms or molecules with a well-defined size varying from a few constituents to several tens of thousands. Clusters are distinguished from bulk matter in so far as their properties are strongly affected by the existence of a surface involving a large fraction of the constituents and by the discreteness of their electronic excitations. On the one hand, the finite nature of the number of constituents leads to novel structural and thermodynamic properties with no equivalent in the bulk. On the other hand, clusters bridge the physics of atoms to the physics of bulk matter. Studying thoroughly the physical properties of clusters may shed new light on elementary excitations in solids and liquids.

The physics and chemistry of atomic clusters and nanoparticles constitute a broad interdisciplinary domain. The field is growing fast, as witnessed by the number of publications and conferences or workshops. The directions of growth are numerous. Some involve pure basic science, others are motivated by more applied material science considerations. Within the fast development of new technologies one observes an unavoidable trend toward miniaturization in micro- and nano-electronics. One wishes to technologically master devices of sizes so small that their quantum specific properties are the most important. Specific magnetic properties of clusters or dots on surfaces might offer new materials for applications in high-density recording and memory devices. Similar trends are observed in other fields, such as catalysis, energy storage, and control of air pollution.

The present school was focused on basic science. It gathered lecturers with research practice in atomic and molecular physics, condensed matter physics, nuclear physics, and chemistry and physical chemistry, not to mention computational physics.

The field has developed rapidly thanks to a strong coupling between theory and experiment. Two predominantly experimental courses provided the opportunity to appreciate what is and will be experimentally possible. Patrick Martin presented a large experimental review, and Hellmut Haberland lectured on recent experimental observations of phase transitions in metal clusters.

The theoretical courses covered three main domains: (i) electronic properties of metallic clusters and nanostructures, (ii) phases and phase changes of small systems, and (iii) chemical processes in nanoscale systems. George Bertsch gave a series of quite interactive lectures that introduced the students to basic phenomena in metal clusters, quantum dots, fullerenes and nanotubes. He presented the basic theoretical tools to study cluster properties, particularly electronic excitations. He emphasized the importance of simple models that large-scale *ab initio* calculations validate, as well as the universal features of finite quantum systems.

The Density Functional Theory stands at a central position as a quantum mechanical method for practical studies of large molecules and clusters. Today, the combination of quantum mechanics and molecular mechanics using classical force fields allows us to understand biological systems to a large extent. Denis Salahub gave the state of the art of this theory, which he illustrated with chemical applications throughout his course.

Metal clusters and nanosystems are excellent physical objects for illuminating the links between the quantum and classical worlds. Matthias Brack reviewed semiclassical methods of determining both average trends and quantum shell effects in the properties of finite fermionic systems. His course was centered on two important theoretical themes: (a) the Extended Thomas–Fermi Model, and (b) the Periodic Orbit Theory (POT).

Pairing correlations in atomic nuclei are intimately related to the phenomena of superconductivity (and superfluidity) in macroscopic systems. Recent experiments on small metallic clusters also reveal pairing correlations. Hubert Flocard devoted his course to a thorough investigation of pairing correlations in finite systems within the state of the art theoretical models.

Cluster and nanoparticle physics is also part of condensed matter physics. Matti Manninen focused his course on the physics of nanosystems from the point of view of condensed matter physics, emphasizing concepts and mesoscopic features that are common between finite systems and low-dimensional systems.

Magnetic properties of small systems are very sensitive to the size, structure, and composition of the system. Within a pedagogical four-lecture course Gustavo Pastor provided a detailed account of the most powerful theoretical methods for efficiently describing the magnetic properties of clusters, particularly transition-metal clusters. The spin-fluctuation theory is quite appropriate for clusters since changes or fluctuations of structure are important. Scattering processes are also useful to gain insight on the many-body properties of finite systems, as demonstrated by Andrey Solov'yov in his two-lecture course. He emphasized the essential role of surface and volume plasmon modes in the formation of electron energy loss spectra.

The thermodynamical properties of clusters are certainly of major importance. They require theoretical approaches to the concepts of melting, freezing and phase changes in finite systems and their dependence on size. The notions of "phase-like" forms, coexistence, solid–liquid equilibrium, phase diagrams and their specific formulation in terms of the thermodynamical variables and functions in various ensembles require the development of new and sophisticated algorithms.

Computer simulations of cluster dynamics and thermodynamics have become a major tool for predicting and understanding the finite temperature behavior of clusters. David Wales' course was concerned with concepts and recent methods of achieving topological analysis and sampling of complex multi-dimensional potential energy landscapes.

Sergei Chekmarev described a novel approach to the computer simulation study of a finite many-body system that allows one to gain detailed information about this system, including its potential energy surface, equilibrium properties and kinetics. Biomolecules can now be investigated with a high degree of confidence.

The chemical processes in or with gas phase clusters and nanoscale particles are a growing field of cluster science. The key to understanding the properties of various families of atomic clusters lies in the determination and description of the chemical bond. Concepts such as valence and valence change, bond directionality, hybridization, hypervalence, electronic population distribution and charge fluctuation are essential. The course of Pavel Hobza addressed the above concepts, methods and mechanisms. Lucjan Piela focused his lecture (not published here) on cooperativity effects in quantum chemistry. This subject is indeed topical for molecular clusters.

In addition to the main courses that are the contents of this book, there were seminars not published herein. These seminars, that triggered stimulating discussions, were given by Jacqueline Belloni, Stephen Berry, Catherine Bréchignac, Vlasta Bonacic-Koutecky, Frank Hekking, Joshua Jortner, Vitaly Kresin, Richard Lavery, Eric Suraud, and Ludger Woeste.

During the four weeks the lecturers and students got to know each other pretty well. Hopefully every student discovered and shared the excitement that his (her) colleagues from other fields experienced. More practically, one would have realized that some as yet unfamiliar methods could be of great interest for one's own research. The overall organization of the school provided the best conditions to meet these goals. The daily lecture program was kept light, with no more than three main courses and sometimes an extra seminar. This schedule allowed plenty of time for discussions and organizing small working groups. We even observed that some collaborative research work had started. On behalf of all the lecturers and students we would like to dedicate this summer school to the late Professor Walter D. Knight. Walter Knight and his group at Berkeley pioneered the experimental field of cluster beams. His experiments in the 1980s led to major discoveries relating to finite size effects and to a strong revival of cluster physics.

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