

# **Physics and Chemistry of Finite Systems: From Clusters to Crystals**

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# **Physics and Chemistry of Finite Systems: From Clusters to Crystals**

## **Volume I**

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## PREFACE

Recent innovations in experimental techniques such as molecular and cluster beam epitaxy, supersonic jet expansion, matrix isolation and chemical synthesis are increasingly enabling researchers to produce materials by design and with atomic dimension. These materials constrained by size, shape, and symmetry range from clusters containing as few as two atoms to nanoscale materials consisting of thousands of atoms. They possess unique structural, electronic, magnetic and optical properties that depend strongly on their size and geometry. The availability of these materials raises many fundamental questions as well as technological possibilities.

From the academic viewpoint, the most pertinent question concerns the evolution of the atomic and electronic structure of the system as it grows from micro clusters to crystals. At what stage, for example, does the cluster look as if it is a fragment of the corresponding crystal. How do electrons forming bonds in micro-clusters transform to bands in solids? How do the size dependent properties change from discrete quantum conditions, as in clusters, to boundary constrained bulk conditions, as in nanoscale materials, to bulk conditions insensitive to boundaries? How do the criteria of classification have to be changed as one goes from one size domain to another?

Potential for high technological applications also seem to be endless. Clusters of otherwise non-magnetic materials exhibit magnetic behavior when constrained by size, shape, and dimension. Nanoscale metal particles exhibit non-linear optical properties and increased mechanical strength. Similarly, materials made from nanoscale ceramic particles possess plastic behavior. Recent discovery of C<sub>60</sub> buckyballs and micro-tubules of graphitic carbon and their ease of production show promise in a variety of industrial applications starting from drug delivery to lubricants and superconductivity. The strong dependence of cluster size on their reaction with reagent gases opens new doors for understanding catalysis. Since the properties of clusters can be drastically modified by changing only a few atoms, one can imagine having a three-dimensional periodic table of elements (cluster size providing the third dimension) from which new materials can be custom made. The field, therefore, represents a true interdisciplinary forum that needs coordinated efforts by physicists, chemists, material scientists, and engineers to tap its full potential in aiding our fundamental knowledge and quest for new materials.

The Physics and Chemistry of finite systems consisting of clusters, nano-structures, and quasicrystals was the subject of a recent international symposium held in Richmond, Virginia during the week of October 8-12, 1991. The purpose of the symposium was to bring together researchers from different disciplines including Physics, Chemistry, Mathematics, materials science, and Engineering to discuss the various challenging problems of both fundamental and technological importance. The symposium consisted of fourteen plenary sessions and two poster sessions. There were fifty two invited papers and 211 contributed poster presentations presented by nearly 300 scientists from 28 countries. The symposium concluded with a panel discussion on outstanding problems and future directions of the field. The proceedings of this symposium constitute this book.

The discussions and presentations included a number of topics:

- Preparation and characterization
- Atomic and electronic structure
- Stability and fragmentation
- Electronic, optical, magnetic, and thermodynamic properties
- Molecular dynamics simulation
- Melting
- Cluster reactions and catalysis
- Cluster support interaction
- Cluster assemblies
- Cluster materials involving C<sub>60</sub> fullerenes
- Technological applications

The symposium was in the planning stage for nearly two years, and we owe our gratitude to a large number of colleagues and institutions who have assisted with the organization of the meeting. We are indebted to Professor Linus Pauling for serving as the honorary chairman of this conference and to members of the International Advisory Board for their help in selecting the topics and speakers. We are grateful to the members of the Local Organizing Committee for spending countless numbers of hours during the planning stage. We wish to thank the conferees for the high quality of their participation in the invited and poster presentations, and exchange of ideas. Our special thanks go to Ms. Barbara Martin for her tireless effort in looking after all the arrangements.

This symposium was made possible by generous grants from the North Atlantic Treaty Organization and Philip Morris, U.S.A. The symposium was also supported in part by grants from the National Science Foundation, Office of Naval Research, Oak Ridge Associated Universities, Army Research Office, and Extrel Corporation. We acknowledge, with gratitude, financial assistance from Virginia Commonwealth University, the symposium host.

P. Jena  
S. N. Khanna  
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## **Volume II**

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