Foreword

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Recent advances in theoretical models, such as density functional theory, and the development of new high speed computing capabilities have made it possible to calculate the properties of a wide variety of molecular species. Atomic and molecular clusters have posed some of the greatest challenges to the understanding of the structures of clusters and their bonding. Today, modern computational methods can provide rational and accurate explanations of the structures and properties of known molecules and can reliably predict the properties of hypothetical ones. Cluster science is one of the frontiers for this rapidly developing technology. Accordingly, we have organized this special issue of the Journal of Cluster Science to provide some examples of the latest research achievements in this area. We have invited a number of the pioneers in this field to contribute to this special issue, and we are very pleased by their response. Contributions have ranged from the studies of the structures of gold clusters to activation of small molecules such as oxygen, hydrogen and furan on platinum-cobalt, ruthenium and iron clusters respectively. We hope this issue will inspire others to use these new methods to advance their own research.

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