Preface

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This special issue of *J. Cluster Sci.* is entitled “*Clusters—from fundamental structures and bonding to electronic, magnetic and catalytic properties*”. During the past four decades, clusters have been focus of intensive studies to understand the evolution from microscopic atoms/molecules to macroscopic condensed matters. The fundamental problems of cluster science lie in the determination of ground state structures of clusters and the exploration of electronic properties as a function of cluster size and structure. To advance the applications, the magnetic and catalytic properties must be thoroughly addressed.

This thematic issue contains ten papers, covering different aspects of cluster research, such as ground state structure, plasmonic resonance, phase stability, melting behavior, electronic and magnetic properties, gas adsorption, and catalytic properties. The systems studied include elementary clusters, metal oxide clusters, binary alloy clusters, and Mn_{12} benzoate. To present a quick overview of this special issue, in the following we briefly summarize these papers.

In “Plasmonic Resonance in Sodium Clusters: Competition Mechanism Between Electron Spill-Out Effect and Quantum Pressure in Electron Gas”, C. Huang investigated the plasmonic resonance of sodium clusters using a generalized non-local optical response theory. The competition between the effects of electron spill-out and quantum pressure in the electron gas has been clarified in terms of the electron spill-out thickness as well as the cluster radius.

In “Structural Evolution of Medium-Sized Phosphorus Clusters (P_{20} – P_{36}) from *Ab Initio* Global Search”, L. Sai et al. determined the ground state structures of medium-

sized phosphorus clusters, P_n ($n = 20$ – 36) by using the comprehensive genetic algorithm combined with DFT calculations. They revealed the essential building subunits for assembling the phosphorus cluster structures. Odd–even oscillations in the size-dependent binding energy and HOMO–LUMO gap of these phosphorus clusters have been discussed.

In “Molecular Interaction, Antimicrobial, Antioxidant, Cytotoxic and Magnetic Properties of Mn_{12} Benzoate”, M. K. Ghosh et al. have reported the synthesis, crystal structure, antimicrobial activity, cytotoxic effect on root tip of *Allium cepa* Linn, antioxidant and magnetochemical properties of $[\text{Mn}_{12}\text{O}_{12}(\text{PhCO}_2)_{16}(\text{CH}_3\text{OH})_4] \cdot 3\text{CH}_3\text{CN}$ cluster. The molecular interaction of Rhodamine B with Mn_{12} benzoate was characterized by the change of UV–Vis absorption peak. The antioxidant activity of Mn_{12} benzoate was assessed by 2,2'-diphenyl-1-picryl hydrazyl radical assay. Variable-temperature and -field solid-state dielectric current and alternative current magnetic susceptibility measurements were performed on the cluster complex.

In “High Coverage CO Adsorption on Fe_6O_6 Cluster Using GGA + U”, X. Yu and co-workers considered a Fe_6O_6 cluster adsorption with 1 to 12 CO molecules using GGA + U calculations. The adsorption mechanism of CO on the Fe_6O_6 cluster has been analyzed and compared with that on Fe_3O_4 surfaces and other iron oxide clusters. Phase diagrams of CO adsorption on Fe_6O_6 have been constructed using atomic thermodynamics.

In “Structural and Electronic Properties of Nano-brass: Cu_xZn_y ($x + y = 11$ – 13) Clusters”, Cheng’s group have determined the equilibrium structures of Cu–Zn alloy clusters with 11 to 13 atoms using genetic algorithm combined with DFT calculations. The structural evolution diagrams that depend on the relative energy are plotted. The molecular orbitals of some spherical-like Cu–Zn alloy clusters with 18 or 20 valence electrons have been analyzed to identify the stable superatoms within the picture of jellium model.

In “Effect of Size and Composition on the Structural Stability of Pt–Ni Nanoalloys”, Y. Yang et al. determined the equilibrium structures of Pt–Ni alloy clusters with

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different sizes (38, 55, 147, 309 atoms) and compositions using genetic algorithm combined with empirical Gupta potentials. Icosahedron structures were found to be the most stable structure for Pt-Ni binary clusters. Further, the effect of composition on the structural stability of Pt-Ni alloy clusters has been discussed.

In “Theoretical Study on the Structural, Thermal and Phase Stability of Pt–Cu Alloy Clusters”, C. Che et al. performed a systematic atomistic investigation on the Pt–Cu nanoclusters with various atomic arrangement, morphologies and sizes based on empirical Gupta potentials. The tendency of distribution of Pt and Cu atoms on surface or inner core sites has been clarified. The melting points and phase diagrams of binary Pt–Cu nanoclusters with different morphologies and sizes have been obtained.

In “Solar Driven CO₂ Hydrogenation on Ti-Doped Silicon Nanocages”, Zhou’s group has theoretically investigated the Ti-doped silicon cage clusters (TiSi_{*n*}, *n* = 12–16) for CO₂ hydrogenation utilizing sun light as energy source. Their first-principles calculations demonstrated that the activity and product selectivity of TiSi_{*n*} clusters can be tailored by cluster size. The origin of chemical activity has been revealed and a relationship between binding capability of TiSi_{*n*} clusters and the *p* orbital center of silicon cluster has been established.

In “Theoretical Investigations on the Nanowires Assembled by the V₁@Si₁₂ Clusters”, Q. Liu et al. have theoretically designed a series of one-dimensional

nanowires assembled by V₁@Si₁₂ clusters. The structures, stabilities, magnetic and electronic properties of these V₁@Si₁₂-based nanowires were examined using DFT calculations. The strain effects on the magnetic and electronic properties of V₁@Si₁₂-based nanowires and the extension to V₃@Si₁₂ and Ti₁@Si₁₂ nanowires have also been discussed.

In “Structural and Electronic Properties of Small Stoichiometric (Li₂O₂)_{*n*} Clusters and Relevance to Li–O₂ Batteries”, S. Lei and co-workers studied the stoichiometric (Li₂O₂)_{*n*} clusters (*n* = 1–6) using DFT calculations. The most stable structures, favorable spin states, and electronic properties (such as HOMO–LUMO gap, frontier molecular orbitals, and photoelectron spectra) of these clusters have been obtained. The theoretical results may have implications for the formation and decomposition of peroxide lithium in lithium air batteries.

The purpose of this special issue is to highlight some recent developments in cluster science within a limited scope. We hope that it will serve as a platform for exchange of innovative ideas in this rapidly growing field and that new and exciting research will emerge from this dialogue.

Finally, we would like to acknowledge the excellent contributions by the authors which make this special issue possible. We are also grateful to the reviewers for their critical and constructive comments.