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PREFACE

Preface

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This special issue of *J. Cluster Sci.* is entitled *Magnetic Clusters and Nanoparticles*. Magnetic nanoclusters are of fundamental and technological importance. Magnetic clusters and nanoparticles are aggregates of a few to thousands of atoms or molecules that exhibit magnetism. Understanding the evolution of magnetism from individual atoms (which obey Hund's rule) to bulk solids (whose behavior is determined by the spin-polarized band structure of the itinerant electrons) through the intermediate stage of clusters is interesting both from the viewpoint of fundamental condensed matter physics as well as that of cluster chemistry. Magnetic clusters and nanoparticles are highly promising materials in many technological fields, such as spintronics, high-density information storage, quantum computing, and magnetic resonance imaging.

This thematic issue contains 4 reviews and 15 original research papers, covering a wide variety of topics dealing with magnetic clusters and nanoparticles. The systems studied include atomic clusters, bimetallic clusters, metal doped carbon and silicon fullerenes, atomic chains, alloy nanoparticles, metal oxide nanoparticles, and compound nanoparticles with or without ligands. To provide our readers with a

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quick overview of these papers, we briefly summarize below what this special issue covers.

There are ten invited articles, including four reviews and six original research papers in this issue. All of them focus on the fundamental issues with regard to the magnetic behaviors of clusters, but each dealing with a different kind of magnetic cluster system.

In the invited review entitled "Magnetism in simple metal and 4d transition metal clusters," P. Sen discusses two aspects of magnetism in small metal clusters: (1) simple metal clusters that are well-described by electronic shell models and mimic properties of elemental atoms, and obey Hund's rule of maximum spin multiplicity; (2) small clusters of 4d transition metal atoms that are non-magnetic in the bulk, but may have magnetic ground states. The known results on Rh clusters are discussed in detail.

In the invited review entitled "Magnetic properties of Pt-based nanoalloys: A critical review," D. Cheng and co-workers review experimental work on the synthesis, characterization, and magnetic properties of Pt-M (M = Fe, Co, or Ni) magnetic nanoalloys, as well as the recent theoretical work on these clusters. Their applications in the fields of biology, information storage, and magnetic separation are also discussed.

In the invited review entitled "First-principles calculations of magnetism in nanoscale carbon materials confining metal with *f* valence electrons," Z. Wang and co-workers outline their first-principles calculations on various nanoscale carbon materials confining U and Gd, which are representatives of the actinides and the lanthanides, respectively. The complex interactions between *f* electrons and *s-p* electrons make the induced magnetic property sensitive to metal species and carbon confinement. Magnetic coupling between metal and carbon structures is also discussed.

In the invited review entitled "Magnetic Silicon Fullerenes: Experimental Exploration and Theoretical Insight", Y. Liu and co-workers summarize progress on silicon clusters with encapsulated metal atoms, with particular focus on the recent identification of magnetic silicon fullerenes. Endohedral doping with rare-earth atoms can stabilize the Si_{20} cage by forming $R@Si_{20}$ fullerene cages. Among them, $Eu@Si_{20}$ had been reported to yield a stable magnetic silicon fullerene. In addition, based on a stable Eu_2Si_{30} tube, a magnetic silicon nanotube had been constructed. These magnetic silicon fullerenes and nanotubes have potential applications in the fields of spintronics and high-density magnetic storage.

In the invited paper entitled "Structure and Spin-polarized Transport of Co Atomic Chains on Graphene with Topological Line Defects," J. Wan and co-workers perform density functional theory (DFT) calculations to explore the nucleation growth of Co atoms absorbed on graphene with extended linear defect (LD@Gr). They predict a patterned growth of linearly arranged Co clusters along the LD. Moreover, the spin-polarized transport properties of the Co/LD@Gr are investigated. This quasi-1D Co/LD@Gr heterostructure, with the polarized spin current parallel to the LD, is suggested as a candidate for future spintronic applications.

In the invited paper entitled "A one dimensional 3d-4f heterometallic chain based on Gd3+ nodes and tetranuclear {Cr4(hdpta)2} complex ligands: synthesis, structure and magnetic properties," J. J. Zhang and co-workers report that the assembly reaction of 1,3-diamino-2-hydroxy-propane-N,N,N′,N′-tetraacetic acid (H_5hdpta), sodium acetate (NaAc), and Cr^{3+} ion at pH 6.7 in aqueous solution leads to the formation of $Na[Cr_2(hdpta)(Ac)_2]$ (**1**). Further assembly of **1** with Gd^{3+} ions give rise to $[Gd(NO_3)_3(H_2O)_4][Cr_4Gd(hdpta)_2(OH)_4(H_2O)_5]\cdot(NO_3)\cdot 32H_2O$ (**2**). Compound **1** bears a 3D (4, 4)-connected ion framework based on mononuclear Na^+ nodes and dinuclear [Cr2(hdpta)$(Ac)_2$]—complex ligands in which two Cr^{3+} ions are chelated by one $hdpta^{5-}$ and also bridged by two acetate auxiliary ligands, while the $[Cr_4Gd(hdpta)_2(OH)_4(H_2O)_5]^+$ monocation **2** exhibits a 1D chain structure based on dianionic $[Cr_4(hdpta)_2(OH)_4]^{2-}$ complex ligands and mononuclear Gd^{3+} nodes. Compound **2** shows overall antiferromagnetic interaction.

In the invited paper entitled "Insight into the relationship between structural and electronic properties of bimetallic Rh_nPt_{55-n} (n = 0–55) clusters with cuboctahedral structure: DFT approaches," S. Huang and co-workers investigate the structural, magnetic, and electronic properties of bimetallic Rh_nPt_{55-n} (n = 0–55) clusters with cuboctahedral structure using DFT calculations. They find that the Pt atoms tend to segregate on the surface, while the Rh atoms prefer to be in the core. The ordered core–shell structure, $Rh_{13}@Pt_{42}$, is found to possess particularly low excess energy. Compared to pure Rh_{55} cluster, the total magnetic moments of bimetallic Rh_nPt_{55-n} clusters are weakened.

In the invited paper entitled "Structural, energetic, and magnetic properties of $Ag_{n-m}Rh_m$ and Ag_mRh_{n-m} clusters with $n \leq 20$ and m = 0 or 1," M. Springborg and co-workers determine the global minimum energy structures of bimetallic $Ag_{n-m}Rh_m$ and Ag_mRh_{n-m} clusters by using a genetic algorithm in combination with either the parametrized density-functional tight-binding method or a Gupta-potential, re-optimized with first-principles calculations. They demonstrate that the exchange of a single silver atom by rhodium leads to compact core–shell-like structures with structural motifs known from the Lennard-Jones clusters. The total magnetic moment of both cluster systems is mainly due to unpaired electrons on the rhodium atoms with a small ferromagnetic contribution from the silver host in $Ag_{n-1}Rh$ and virtually no contribution to the total magnetic moment from the single silver atom.

In the invited paper entitled "Magnetic anisotropy of small Ir_n clusters (n = 2–5)," X. Q. Liang et al. calculate the magnetic anisotropy energies (MAEs) of small Ir_n clusters of up to five atoms by employing a noncollinear implementation of DFT including spin–orbit coupling (SOC) interaction. They find that SOC leads to formation of large orbital moment and a mixing of different spin states, but does not affect the relative stability of different structural isomers for a given cluster. The MAEs obtained from DFT calculations are further supported by the analysis of torque approach.

In the invited paper entitled "Deposition Morphology and Magnetism of Co, Pt Adatoms and Small CoPt Adclusters on Ni(100) Substrate," H. Yuan and co-workers use DFT with SOC to calculate the spin and orbital magnetic moments, as well as the MAE of small CoPt clusters with up to three atoms on Ni(100) surface.

They find that the ferromagnetic Co atoms in intra CoPt adclusters couple ferromagnetically with the underlying Ni atoms. The predominant "inter-interactions" between Co adatoms and Ni surface, together with the secondary "intra-interactions" between Co adatoms and Pt adatoms, lead to a strongly quenched orbital moment but a less quenched spin moment. The MAEs of CoPt adclusters exhibit a strong dependence on alloying effect. The oxidations of CoPt clusters always reduce orbital magnetic moments and consequently decrease the corresponding MAEs.

Also included in this issue are nine contributed research papers.

We hope that this special issue will serve as a platform for exchange of innovative ideas in the sub-field of *magnetic clusters and nanoparticles* and that new and exciting research will emerge from this dialogue.

Finally, we wish to acknowledge the important contributions of the authors and the tireless efforts of the reviewers who have made this special issue possible.