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REVIEW

Effects of 5f-electrons on electronic structures and superatomic

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5f-elements encaged in gold superatomic cluster are capable of giving rise to unique optical properties due to their hyperactive valence electrons and great radial components of 5f/6d orbitals. Herein, we review our first-principles studies of 5f-elements encaged gold superatomic clusters with different dimensions. The three-dimensional (3D) Ac@Au$_{12}$ and Pa@Au$_{12}$ clusters possess the 18-electron configuration of $1S^21P^61D^{10}$ and 19-electron configuration of $1S^21P^61D^{10}2S^1$, respectively, importantly, the 5f/6d orbitals involved in surface-enhanced Raman spectroscopy (SERS) spectra for 3D and 2D structures in both the bonding and antibonding orbitals, providing the enhancement factors of the order of $\sim 10^5$ at 488 nm and $\sim 10^6$ at 456 nm, respectively. This work implies that the superatomic orbital transitions involved in 5f-elements can not only lead to a remarkable spectroscopic performance, but also a new direction for optical design in the future.

Keywords: 5f-electrons, ds-electrons, superatom, first-principles

PACS: 31.70.–f, 32.30.–r, 36.40.–c, 71.15.Rf **DOI:** 10.1088/1674-1056/25/8/083102

1. Introduction

Gold nanoparticles exhibit strong d–s hybridization and relativistic effects which results in a wide variety of optical phenomena. These properties have attracted a huge interest in the optical studies of bimetallic nanoparticles.[1–9] On the one hand, the [illegible] narrow and sharp in the visible range,[10–12] and these spectra index could be hardly influenced by the external coordination environment.[13–15] On the other hand, the [illegible] comprised of f-block and ds-block elements could be envisioned to very likely carry a revolutionary spectroscopic performance.

One of the first superatomic experiments was the seminal [illegible] electrons. This particular attribute has led to an intense interest in optics and magnetic fields in applications of f-element-embedded gold clusters, such as Ac@Au$_{12}$,[17] Sg@Au$_{12}$,[18] [illegible] Specific optical characteristics of these superatom models were obtained through their structural and compositional modifications.[26–34] The relevant modification produces spectra shifting in a very wide range that is even as important as the morphological modification in one component [illegible]

modeled via the superatom models.[14–18] The first predicted superatomic cluster was the icosahedral [illegible] density functional theory (DFT) involving the 18-electron count ($1S^21P^61D^{10}$),[19] which was later [illegible] them, these superatomic clusters all possess a great advantage compared with the pure gold clusters in tuning the excitation energy and two-photon optical absorption,[41,42] circular dichroism [illegible] can be effectively explained by superatom models.

As is well known the f-block elements have a h [illegible] ous peaks in the mass spectra [illegible] 20, 40, [illegible] atoms. The electron [illegible] fined in quantized orbitals $1S^2$ [illegible] electronic shell structure [illegible] the magic clusters. Subsequ [illegible] lowing as well as the aromati [illegible] the relationship between electr [illegible] stability.[14] Currently, the elect [illegible]

tural Science Foundation of China (Grant No. 11374004), the Science and Technology Development Program of Jilin [illegible] 21JH), the Fok Ying Tung Education Foundation, China (Grant No. 142001), and the Support from the High Performance [illegible] Center, China.

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Journal of Materials Chemistry A

PAPER

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Carbon-coated $Na_3V_2(PO_4)_2F_3$ nanoparticles embedded in a porous carbon matrix as a superior cathode material for sodium-ion batteries

Haofei Bie,[c] [illegible] Xu Yang,[a] Nan Chen,[a] Chunzhong Wang,[ab] Xi [illegible]

A carbon-coated $Na_3V_2(PO_4)_2F_3$ nanocomposite (NVPF@C) is successfully realized by a facile sol-gel method. Carbon-coated NVPF nanoparticles are well-dispersed in the three-dimensional carbon matrix, which [illegible]. As a result, the NVPF@C nanocomposite demonstrates remarkable Na-storage performance, delivering a high reversible capacity of about 120 mA h g^{-1} over 50 cycles between 1 and 2.6 V, superior rate capability with specific capacities of about 77 mA h g^{-1} at a high current density of 5 C (1 C = 132 mA g^{-1}) and long-term cycle life with capacity retentions of 70% and 50% over 1000 and 2000 cycles at 10 C and 30 C rates. Thanks to the moderate high energy and power densities, the NVPF@C nanocomposite is suggested as a promising cathode material for grid energy storage.

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Introduction

Recently, sodium-ion batteries (SIBs) for grid energy storage have attracted to the natural abundance and low c[illegible] SIBs share the identical [illegible]

performance, preparing nanocomposites with carbon-related materials such as one-dimensional carbon sheaths,[9,10] sprouts,[11] as a promising candidate,[12] carbon CMK-3,[13] nanothorns,[14] and core-shell structures,[15] is d worldwide interest owing employed as an effective strategy to particular, Mai *et al.*[16] ost of sodium.[17] In particular, studied the effect of carbon matrix dimensions on the proper[illegible] ercalation chemistry with [illegible] of NV_2 nanosheets and found that the NV_2/acetylene

(Na super-ionic conductor) structure have received particular attention because the three-dimensional open framework gives rise to plenty of interstices capable of allowing fast Na^+ insertion and extraction with little lattice strain.[18] $Na_3V_2(PO_4)_3$ (NVP), as a widely studied cathode material with a NASICON-type structure, has been found to demonstrate attractive Na^+ storage properties both at high and low working potentials.[19] However, its low electronic conductivity still hinders the rate capability and long-term cycle life, which are considered as two critical characteristics for SIBs to realize Na^+ storage

increased the electronic conductivity but also provided the robustness for the structure during cycling.

Fluorophosphate $Na_3V_2(PO_4)_2F_3$ (NVPF) is known as another appealing NASICON-type material, exhibiting moderating intercalation chemistry for both Na^+ and Li^+ ions.[20] Basically, NVPF can be considered as using three F^- to replace one $(PO_4)^{3-}$ polyanion of NVP to maintain the charge neutrality. However, NVPF crystallizes in tetragonal symmetry with a space group of $P4_2/mnm$, in sharp contrast to the rhombohedral symmetry of NVP (space group $R\bar{3}c$).[21] NVPF is built up with $V_2O_8F_3$ bioctahedral units alternately bridged by PO_4 tetrahedral units, which forms an open three-dimensional framework with large tunnels along [110] and [1$\bar{1}$0] directions in the crystal structure. Because a configuration reference to the [illegible] is introduced.[22] Also, the inductive effects of the $(PO_4)^{3-}$ polyanion might be enhanced due to the strong ionicity of the

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search Article

Actinide embedded gold superatom models: Isoelectronic structure, spectroscopic properties, and applications in surface enhanced Raman scattering

[redacted]

Actinide elements encased in a superatomic cluster can exhibit original [redacted] spectroscopic properties of $Th@Au_{14}$ are predicted and compared with that of the isoelectronic entities $[Ac@Au_{14}]^-$ and $[Pa@Au_{14}]^{2-}$ using density functional theory. The calculation results indicate that these clusters all adopt a closed-shell superatomic 18-electron configuration of the $1S^21P^61D^{10}$ Jellium state. The absorption spectrum of $Th@Au_{14}$ can be interpreted by the Jellyumatic orbital [redacted] laser band exhibit strong peaks attributable to charge transfer (CT) from the metal to the pyridine molecule. These charge transfer bands lead to a resonant [redacted] scattering

KEYWORDS
actinide element,
DFT calculation,
gold nanoparticle,
superatomic orbital,
[redacted]
scattering

[redacted]al, electronic, and magnetic properties of these [redacted] encapsulated atoms can also be modified in order to atten- satisfy specific requirements in the design and fabri- [1–3] cation of cluster-based functional nanomaterials [4–9]. oms Interestingly, many stable endohedral gold clusters the have been characterized by specific "magic numbers" rates of valence electrons consistent with atomlike electronic

1 Introduction

The optic

Hollow gold clusters have received substantial tion in recent years in studies of metallic clusters because of their ability to house foreign guest at and molecules. Encapsulated atoms can affect formation of gold clusters and their agglome

[redacted]
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