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### **EDITORIAL**

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## Introduction to nanoclusters: from theory to application

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Since C<sub>60</sub> was first successfully prepared in the 1980s, the vigour of nanoclusters has spurred wide applications in electronics, energy storage, catalysis, biosensors and nanomedicines, etc. Ultra-small size and unique structures are the key for their distinct properties. Conventionally, spectroscopic experiments, such as photoelectron spectroscopy, combined with the firstprinciples calculations have been proven to be a powerful tool for determining the structures in vacuum and the gas phase. Since the millennium, significant progress has been achieved in synthesizing clusters with specific morphologies and/or atomic structures in liquid, which prompts the preparation of nanoclusters in large amounts and tunes their properties to atomic precision. This kindles intense interest in the fundamental understanding of the evolution of the structures of nanoclusters and their corresponding structureactivity relationships.

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On this specific theme, we present 16 articles, ranging from basic research, such as the study of atomic structures and the interaction between the clusters and other materials, to their precise synthesis, and further extend to the applications in a variety of frontier areas, including optics, biomedical imaging, the semiconductor industry, etc.

#### Structures

Characterizing the structures of clusters lays the bedrock to understanding their properties and applications. Wang et al. combined the state-of-the-art spectroscopy techniques with quantum chemical calculations to reveal the structures and size effects of H2O-metal clusters (https://doi.org/10.1039/D3NA00873H). Ji al. designed the metallocene nanowires in different shapes and predicted their magnetic and electronic (https://doi.org/10.1039/ characteristics D3NA00926B). Cai et al. introduced a machine-learning method to construct the high-dimensional neural network to resolve the complexity of the configurational space of cerium oxide clusters (https://doi.org/10.1039/ D3NA01119D). Han et al. applied the grand unified model to predict three medium-sized ligand-protected clusters and further confirmed their thermal/chemical stabilities and optical spectra by using density functional

calculations (https://doi.org/ theory 10.1039/D3NA00372H).

#### Interaction

Li et al. applied molecular dynamics simulations to show a gold surface could induce the conformational change of proteins (https://doi.org/10.1039/ D3NA00185G). Fouegue et al. theoretically demonstrated the drug delivery potential of pure/doped C<sub>24</sub> fullerene (https:// doi.org/10.1039/D3NA00402C).

### Synthesis

Clusters synthesized with different structures exhibit different properties. Miliaieva et al. demonstrated the distinct electronic characteristics of nanodiamond clusters according to the different synthesis methods used (https://doi.org/ 10.1039/D3NA00205E). Schmitt et al. presented a novel method to the fully scalable, continuous flow synthesis of atom-precise Pt nanoclusters (https:// doi.org/10.1039/D4NA00074A). Pluta et al. and Veedu et al. reported the methods to quantum dots presenting synthesize enhanced NIR photoluminescence (https://doi.org/10.1039/D3NA00404J, https://doi.org/10.1039/D3NA00869J). Vu et al. reported a facile way to synthesize alloys with improved surface-enhanced Raman scattering performance (https:// doi.org/10.1039/D3NA00483J).

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## **Applications**

The discrete energy levels of nanoclusters provide the versality to tune their optical, electronic, and chemical properties, which are important for their applications. Xia *et al.* took advantage of the chemo-photothermal effect by lightinitiated aggregation of gold nanoparticles for tumor therapy (https://doi.org/10.1039/D3NA00114H). Superresolution bioimaging was fulfilled by

using the dual-color core-shell SiO2 nanoparticles (https://doi.org/10.1039/ D3NA00310H). The promoted spin polarization with tunable magnetic properties of nanosized MXene were reported by Vénosová and Karlický (https://doi.org/10.1039/D3NA00474K). Tseng et al. unveiled the capability of Hf clusters to enable high resolution EUV photoresists (https://doi.org/10.1039/ D3NA00508A). Copper hydride clusters catalysts were good for

hydrogenation and reduction reactions (https://doi.org/10.1039/D3NA01145C).

Nowadays, fast development of highresolution characterization methods and artificial intelligence give new opportunities for characterizing the dynamic behaviors of clusters and designing new functional materials, which will witness a prospering era of cluster science and technology.