【Grant-in-Aid for Transformative Research Areas（A）】

Superatomic Materials: Creating Innovative Materials from Artificial Atoms

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Purpose and Background of the Research

●Outline of the Research

Humanity has achieved prosperity by assembling a few dozen elements into diverse functional materials. This conventional strategy relies on the precise arrangement of atoms based on their individual electronic and bonding properties. However, to overcome modern environmental and energy crises, a new paradigm in material creation beyond existing trajectories is essential.

Our focus is on "atomic clusters," ultrafine particles of several to hundreds of atoms. These clusters possess discrete electronic states distinct from bulk materials, harboring extraordinary properties that defy conventional wisdom. As the entire particle behaves as a single "giant atom," we define it as a "**superatom**" (Fig. 1). Its essence lies in the ability to dramatically and freely modulate properties by subtle manipulations of its constituent atoms and geometry.

In this research area, we position superatoms as "next-generation building blocks" to explore vast, previously inaccessible chemical spaces. By designing these novel blocks and precisely controlling their interactions and organization, we aim to facilitate the emergence of advanced functions that transcend individual properties. Ultimately, we seek to establish a new academic foundation that integrates theories of structure, bonding, and properties, while developing innovative materials to address global challenges.

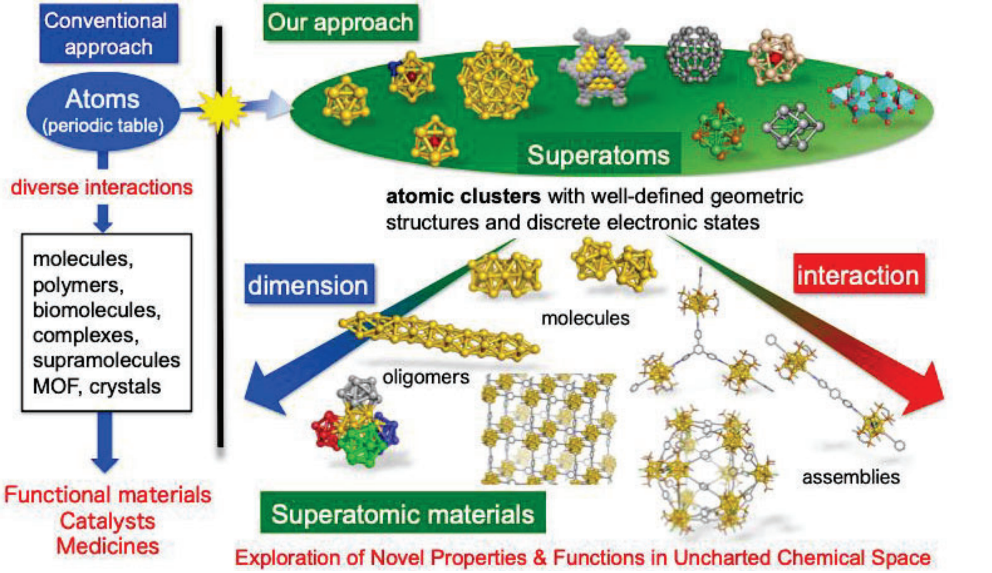

Figure 1. Overview of a new material chemistry based on superatoms as fundamental building blocks.

Expected Research Achievements

●Strategies for Advancing the Research Area

The cornerstone of this project is to expand the “Superatom Library” and develop assembly technologies for creating “superatomic materials” that transcend conventional boundaries. By integrating cutting-edge measurements with theoretical analysis, we will elucidate the mechanisms of underlying functional emergence. The following three research groups will collaborate to achieve the ultimate goal of developing unique superatomic materials based on rational guiding principles (Fig. 2):

A01 (Synthesis): Precision creation of diverse superatoms and their organization into innovative superatomic materials.

A02 (Properties & Functions): Exploration and verification of unique properties and unknown functions inherent in superatomic materials.

A03 (Analysis & Prediction): Elucidation of emergence mechanisms and prediction of novel functions through state-of-the-art measurements and theoretical analysis.

We will also conduct the following collaborative projects to open new frontiers:

- **Optical Energy Conversion:** We aim to realize systems that efficiently convert near-infrared (NIR) light from sunlight into higher-energy visible light utilizing gold superatomic oligomers (termed "gold quantum needles") as sensitizers.
- **Catalytic Functions:** We aim to create superior catalysts for hydrogen evolution and carbon dioxide valorization leveraging unique electronic structures and charge gradients induced through the assembly of superatoms.
- **Stimuli-Responsive Multi-Functions:** We aim to achieve dynamic ion-conductivity control and multi-functional smart materials featuring nanoporous with redox-active superatoms precisely arranged on the inner walls.

●Expected Impact (Fig. 3)

- **Academic Advancement:** We aim to systematize superatoms as a "New Periodic Table" and establish a rigorous foundation for a comprehensive materials science, encompassing theories of structure, bonding, fundamental properties, and reactivity.
- **Human Resource Development:** We will cultivate next-generation leaders with broad, interdisciplinary perspectives capable of transcending the boundaries of existing specialized fields.
- **Societal Contribution:** By driving innovation in fields such as quantum materials, energy devices, and medical technologies, we seek to provide transformative solutions to global challenges.

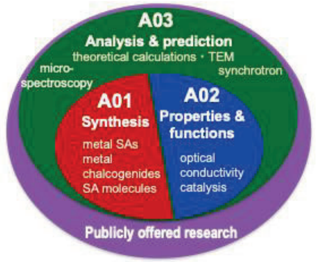

Figure 2. Organization of research groups

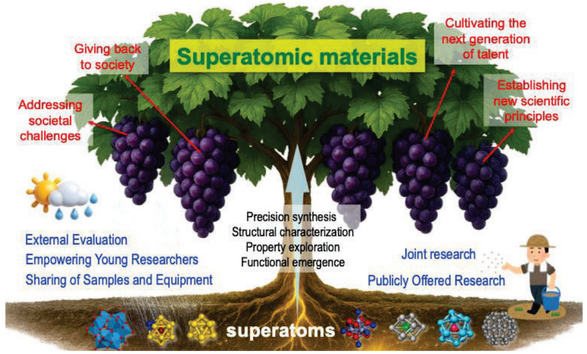

Figure 3. Towards the creation of a new paradigm in materials chemistry

Website(s)	https://www.superatomic-materials.jp/en/ (HP)