Atomically Precise Materials Chemistry for Sustainable Society

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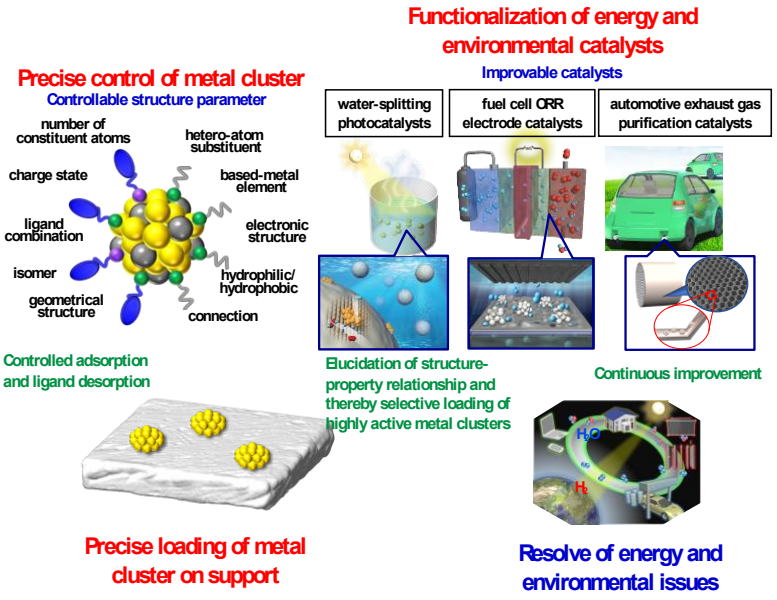
Abstract

The transition to a sustainable society requires materials that can convert renewable electricity into chemical fuels, close carbon and resource cycles, and use precious metals with maximum efficiency. Atomically precise materials chemistry (APMC) provides a powerful route to this goal by controlling the number, composition, geometric structure, and surrounding environment of metal clusters at the molecular level. Such control makes it possible to establish clear structure–property–function relationships and to translate them into practical functional materials.

In this lecture, I will introduce our recent approaches to APMC based on atomically precise metal nanoclusters and cluster-derived nanomaterials. First, precise control of cluster composition, alloying, hydride incorporation, and ligand shells enables the electronic and geometric structures of active sites to be deliberately designed. Second, scalable synthesis and carbon-supported ultrafine platinum nanoclusters provide highly efficient electrocatalysts for hydrogen-related reactions while minimizing Pt consumption. Third, copper nanoclusters with well-defined local coordination environments demonstrate how atomic-scale design can steer electrochemical CO_2 reduction and nitrate reduction toward desired products. Finally, integration of metal clusters with porous frameworks and carbon materials offers new opportunities for selective separation, environmental remediation, and energy conversion.



These examples illustrate how APMC bridges fundamental cluster chemistry and device-oriented materials research. By combining precise synthesis, advanced characterization, theory, and scalable processing, APMC can accelerate the creation of efficient and resource-conscious materials for a sustainable society.

Keywords: atomically precise materials chemistry; metal nanoclusters; electrocatalysis; sustainable energy; resource circulation

References

1. S. Biswas, D.-e. Jiang,* Y. Negishi*, et al., ***J. Am. Chem. Soc.*** 147, 23733−23742, 2025.
2. H. Sakai, Y. Negishi,* T. Hasobe*, et al., ***J. Am. Chem. Soc.*** 147, 13483-13490, 2025.
3. M. Sera, S. Hossain,* Y. Negishi*, et al., ***J. Am. Chem. Soc.*** 146, 29684−29693, 2024.
4. T. Kawawaki, Y. Negishi*, et al., ***J. Am. Chem. Soc.*** 146, 26808−26818, 2024.
5. S. Biswas, B. Pathak,* Y. Negishi*, et al., ***J. Am. Chem. Soc.*** 146, 20937−20944, 2024.