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

Hyperuniform Aperiodic Materials: Pioneering Functions through Control of Vast Potential Structural Degrees of Freedom

Principal Investigator	Sophia University, Faculty of Science and Technology, Associate Professor SAKAI Shiro	Researcher Number : 80506733
Project Information	Project Number : 25B204 Keywords : Hyperuniformity, amorphous, quasicrystals, photonic materials	Project Period (FY) : 2025-2027

Purpose and Background of the Research

●Outline of the Research

While conventional solid-state physics has mainly targeted periodic crystals in which atoms are arranged periodically, there are also solids called quasicrystals, in which atoms are arranged in an aperiodic order, and amorphous materials, in which atoms are distributed irregularly. These aperiodic materials exhibit physical properties distinct from periodic crystals while their aperiodicity has defied a theoretical treatment, giving few guidelines for controlling the properties of these materials. This has prevented them from being fully utilized as functional materials. This Research Area introduces a framework called hyperuniformity (HU) [Torquato and Stillinger, Phys. Rev. E **68**, 041113 (2003)] to classify the structures and electronic states of aperiodic materials, aiming to establish fundamental theories for understanding and controlling their physical properties. Through systematic studies, we strive to maximize the characteristic properties and expand the potential of aperiodic materials (Fig. 1).

●Background of the Research

Periodic crystals are classified by their structural symmetry, which allows a systematic analysis of experimental results and has advanced the theoretical understanding of them. However, periodicity imposes a strong constraint on the structure, and a vast potential lies outside of this constraint. In particular, there are structural degrees of freedom that cannot be distinguished by symmetry. As it is difficult to discuss them all together without classifying them, the theory of aperiodic materials has lagged behind.

The HU framework, which has been developed in the field of statistical physics, classifies and quantifies the regularity of a point distribution in a space. For example, Figures 2(a) and 2(b) are both irregular while the latter is more uniform than the former. A distribution like (b), uniform on a large scale (even if irregular on a short-length scale), is called a hyperuniform distribution. In HU framework, several qualitatively different classes of hyperuniform distributions are defined, as shown in Figure 3.

This research area is a theory-computation-experiment collaborative project that applies HU to aperiodic materials, aiming to establish fundamental theories and develop their applications.

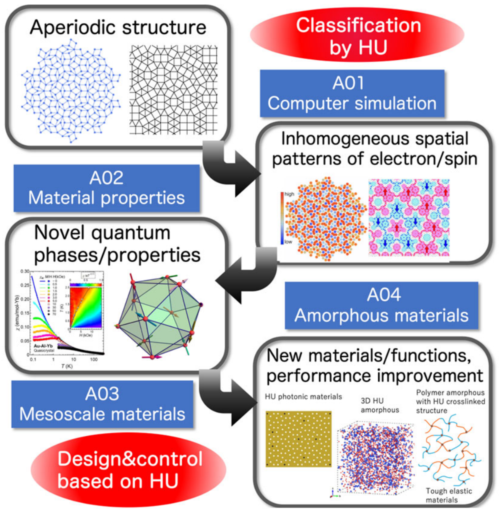

Figure 1. Overview of the Research Area

●Specific Tasks

1. Generation of various aperiodic structures by computer simulation. Construction of neural networks to classify the generated structure in terms of HU.
2. Exploration of novel electron phases in aperiodic materials. Elucidation of the phase transitions between them, and the critical phenomena associated with them.
3. Elucidation of the relationship between the properties and the regularity of their spatial distribution.
4. Theoretical design of aperiodic materials with desirable properties.
5. Realization of the designed structures on a mesoscale using polymer and photonic materials.
6. Exploration of the phase transition between two amorphous phases with distinct homogeneity.
7. Synthesis of 3D hyperuniform amorphous materials.

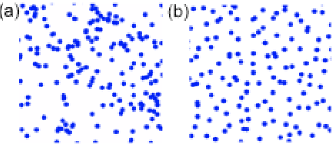

Figure 2. (a) Random distribution. (b) Disordered HU distribution.

Expected Research Achievements

●Goal of the Research Area

Through the HU classification (Fig. 3), we systematically study the properties of aperiodic materials, exploring new material phases, phenomena, and functions by controlling the nonuniform distributions (Fig. 4).

●Goal of each planned research group

A01 Simulation Group (Sakai, Koga): Specific Tasks 1 and 2.
A02 Condensed Matter Group (Sugimoto, Deguchi): Specific Tasks 2 and 3.
A03 Design and Synthesis Group (Takemori, Yamamoto, Ota): Specific Tasks 4 and 5.
A04 Amorphous Materials Group (Stellhorn, Amakai, Ikeda): Specific Tasks 6 and 7.

●Expected ripple effects

Fundamental theory on aperiodic materials will contribute to the social infrastructure through the development of new functional materials. In particular, the disordered HU distribution, possessing both isotropy and homogeneity, could be applied to high-strength materials, soundproofing and heat-insulation materials, highly transparent glass, and energy-saving optical devices using photonic materials. It could also give a new guideline for improving the performance of functional materials such as superconductors, magnets, semiconductors, and solar cells by controlling the spatial distribution of impurities and added atoms.

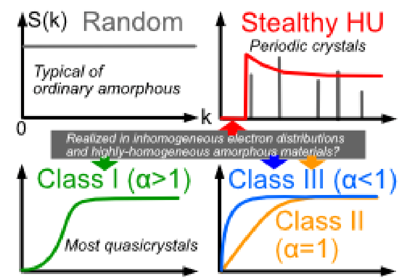

Figure 3. HU classification of structures through the long-wavelength (k~0) behavior of the function S(k) that characterizes the structure.

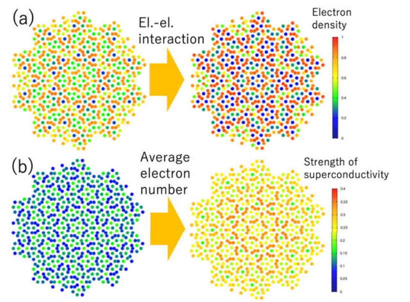

Figure 4. Change of the spatial distribution on a quasicrystalline structure. (a) Electron density varies with the electron-electron interaction strength. (b) Superconducting order parameter varies with the average electron number.

Homepage Address, etc.	https://www.hu-ap-mat.qiqb.osaka-u.ac.jp/english