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

Materials design transformation by understanding non-equilibrium and collective ion flow (Ion Jamology)

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Purpose and Background of the Research

●Outline of the Research

Is it possible to use the analogy of "car traffic" to understand the movement of ions and molecules in chemical reactions? When a Li-ion battery or an all-solid-state battery is charged, ions move from the positive electrode to the negative electrode. This is similar to the traffic flow of cars. In batteries, different factors often obstruct the flow of ions, leading to poor performance.

We refer to this obstruction of ion movement as an "**ion jam**." This issue happens in different reactions, such as battery reactions, catalytic reactions, hydrogen storage, and crystal growth. Therefore, we consider that "jamology," a field of mathematical science that emerged in urban, civil, and traffic engineering, could be applied to resolve this issue.

This study **integrates materials science (batteries and catalysts) and jamology** to establish a new academic paradigm, "**ion jamology**." By understanding and controlling ion jam phenomena, new materials (batteries, catalysts, etc.) will be developed to achieve a carbon-neutral society. Moreover, we will advance mathematical science through new problems emerging from experiments and modeling.

●Collective motion of ions:

Materials Science (batteries and catalysts) x Mathematical Science

We focus on the **interaction between ions** to improve material properties. In recent years, the collective control of ion flow has attracted considerable attention to achieve better properties. In such materials, crystal lattices and aggregates of atoms and molecules (clusters) deform quickly and softly to promote ion flow and enhance their functions.

The current theory is not sufficient to construct a new theory. Conventional theories have assumed that each ion can move independently. This is true only when the ion density is dilute. As ion density increases, the interaction between ions becomes non-negligible. Therefore, it is desirable to construct a theory that appropriately captures the **collective motion of ions**. We will build a new discipline “ion jamology” by combining jamology with quantum chemistry, solid-state chemistry, and solid-state physics.

Jamology is the science that deals with the collective motion and flow of vehicles and people, or in other words, a branch of mathematical science that studies transportation and logistics. It considers vehicles and people as particles and incorporates the interactions among these particles. The fundamental difference between ion jamology and conventional materials and chemistry research is that it incorporates interactions between particles to **describe dynamic processes** and pioneer methods to **control ionic flows** from a broad perspective.

●Management: The Idea Behind the Logo (Fig. 1)

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ion jamology

Figure 1　Logo

1. The nine large cubes represent crystals and composite materials, also showing the plan of this research, which consists of three planned research projects and three fusion research projects. The three planned research projects and the three fusion projects will serve as the weft and the warp, respectively, and all work in unison.
2. The surrounding small cubes represent catalytic reactions and material synthesis processes. They also represent the gathering of researchers and the growth of this research. The management of this domain will be conducted with the utmost importance placed on "**enjoying research**."
3. The ion flow is embedded in the form of an arrow.
   Theoreticians and experimentalists work closely together, conducting **original experiments inspired by theory and mathematical science**. The experimental results are then fed back to theoreticians to create a positive spiral.

Expected Research Achievements

All A01, A02, and A03 research members promote the following three fusion projects. These projects will be the starting point for building up the science on the collective motion of ions and achieving a revolution in "Materials design transformation by understanding non-equilibrium and collective ion flow" for battery and catalyst materials.

1) Ion collective flow (micro- and meso-region)
Experimentally verify the collective motion of ions on a crystal lattice scale using single crystals and model materials.

2) Pathway network (meso-macro domain)
The pathway networks are analyzed using molecular dynamics and dynamic Monte Carlo methods on a wider spatial scale. New materials are synthesized and characterized using advanced synthesis and measurement techniques.

3) Overall optimization (micro-meso-macro domain)
The micro-meso-macro domain is connected by optimizing grain boundary/interface design and composite.

Three planned research projects, led by young leaders, are underway.
A01: Computational Mathematics (Yasunobu Ando, Tokyo Institute of Technology)
A02: Materials Creation (Genki Kobayashi, RIKEN)
A03: Advanced Measurement (Takashi Nakamura, Nagoya Univ.)

Specific materials include H^- and Li-ion conductors. For example, the phase transition of $Ba_{1.75}LiH_{2.7}O_{0.9}$ is expected to involve a combination of ion-ion and ion-lattice correlations and is a unique target of ion jamology. In addition, the ionic conductivity of $Li_{10}GeP_2S_{12}$ (LGPS) will be investigated by state-of-the-art measurement techniques to clarify the diffusion paths and diffusion coefficients of Li ions, and first-principles calculations and mathematical model calculations will be used to establish material design guidelines.

We first focus on battery and catalyst materials, mainly inorganic materials. Gradually, we will expand the scope of ion jamology to various chemical and material fields.

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