

Translating materials with math

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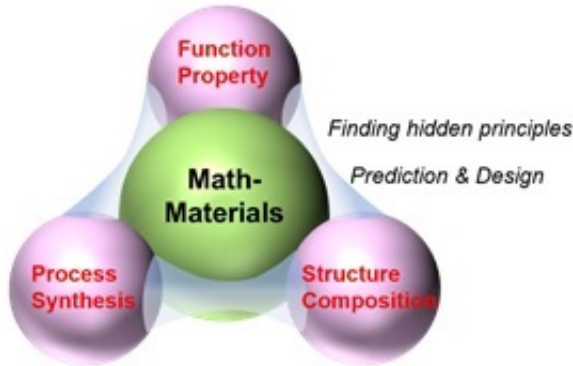


Fig. 1: Mathematics may help relate the structure/composition and properties/functions of materials and suggest novel strategies for their synthesis. Credit: Motoko Kotani & Susumu Ikeda

Mathematics has been very successful throughout history in translating complex scientific concepts. Einstein's famous equation $E=mc^2$, for example, describes how mass and energy are interchangeable. But as scientific fields become increasingly complex and specialized, the "language" of mathematics needs to keep pace to develop the mathematical vocabulary necessary to describe both the knowledge and cumulative experience gained by scientists working in the physical world.

Materials science is a rapidly evolving interdisciplinary field of science that involves the discovery and design of [new materials](#). The field involves understanding the properties and functions of materials at the

atomic/molecular scale as well as the macroscopic scale.

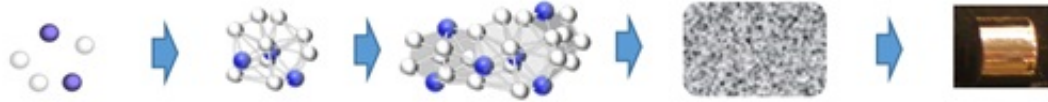
Motoko Kotani and Susumu Ikeda from the Advanced Institute for Materials Research, Tohoku University, Japan, have published a vision article in the journal *Science and Technology of Advanced Materials (STAM)* that emphasizes the need for strong collaboration between [materials scientists](#) and mathematicians to break down the barriers of specialized scientific language and create a comprehensive and common understanding of this highly specialized and subdivided field (Fig. 1).

One potential area for fruitful collaboration, for example, is using discrete geometric analysis (graph theory combined with differential geometry) in the study of [nanoporous materials](#), the researchers explain (Fig. 2). Graphs are mathematical structures made up of nodes connected by lines and are used to describe relationships between objects. Nanoporous materials are being used, for example, as membranes to improve energy-storage in capacitors by removing molecules from around ions as they pass through the extremely tiny pores of these materials. The ability to analyze the three-dimensional structure of these pores is important for understanding their physical and chemical properties. Discrete geometric analysis (or graphs taking geometric features into account) could be a powerful tool to investigate the transport of materials through these tiny structures.

Mathematicians have interacted with scientists in other fields over the course of history. But in the 20th century, they underwent a much-needed time of isolation to develop their field, the researchers explain; "after reaching a satisfactory level of advancement, the field should open its doors to seek inspiration." Efforts to fuse mathematics with science generally and [materials science](#) specifically are gaining momentum. "It is a good time for mathematics and materials science to encounter each other and interact," the researchers conclude.

Discrete geometry

Connection between discrete atoms, clusters, molecules and continuous bulk materials



Extraction of geometrical elements from complicated continuous structures using “graph”



Fig. 2: Examples showing the power of geometry: relations between continuous and discrete elements in materials, and extraction of discrete geometrical elements. Credit: Motoko Kotani & Susumu Ikeda.

More information: Motoko Kotani et al. Materials inspired by mathematics, *Science and Technology of Advanced Materials* (2016).
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