The crucial role of functional motifs—microstructural units that govern material functions—in material research

1 April 2022

The paradigm starts with the main aspects of microscopic structures and the properties of materials. On the basis of which the functional motifs governing the material properties can be extracted and the quantitative relationships between them can be investigated, and the results could be further developed as the "functional motif theory." The latter should be useful as a guideline for creating new materials and as a tool for predicting the physicochemical properties of materials.

The properties of materials are determined by their functional motifs and how they are arranged in the materials, with the latter determining the quantitative structure–property relationships. Uncovering the functional motifs and their arrangements is crucial in understanding the properties of materials, and the functional motif exploration enables the rational design of new materials with desired properties.

In terms of the length scale of structural features, material structure can be classified into macroscopic, mesoscopic, and microscopic structures. And the microscopic structure of materials can be plausibly categorized into six types: (1) crystalline structures possessing a long-range order of atoms, (2) magnetic structures with long-range order of spin moments in crystalline materials, (3) aperiodic structures with long-range organized atom modulations from a crystalline materials, (4) defect structures with long-range random or...
nonrandom distributions of atomic defects in crystalline materials, (5) local structures representing local-coordination environments of atoms in the range of several coordination shells, and (6) electronic structures representing electron density distributions in real space (or position space) and those representing electron distributions in momentum space (or k-space). This classification is not too much rigorous, while it benefits the investigations of functional motifs and structure-property relationships. (Pink balls in red square represent the atoms in a repeat unit cell; black arrow represents spin moments. The blue lines highlight the relative positions of atoms.). Credit: Science China Press

Given the importance of microscopic structures in the functional motif paradigm, it is necessary to fully understand material structures. The hierarchy of material structure involves information crossing multiple length and time scales. Jiang X-M et al classify the material structures into macroscopic, mesoscopic, and microscopic structures, and further classify microscopic structures into six types. i.e., the crystal, magnetic, aperiodic, defect, local, and electronic structures. For each type of microscopic structure, Jiang X-M et al present the role of functional motifs and their arrangements in determining properties with representative functional materials.

Jiang X-M et al take Infrared (IR) NLO materials as an example to introduce the function-oriented design strategy of new functional materials, in which the role of functional motifs of materials is stressed in the design of materials. This strategy differs from the traditional structure-oriented design strategy.

Jiang X-M et al also discuss the important role of high-throughput experimentation and calculation in material studies and the challenges for extracting functional motifs from a huge amount of data on material structures and properties. Machine learning is expected to be useful for efficiently predicting material properties and screening materials with desired properties. For the design of new materials, developing sufficiently reliable material structures and property databases and new effective methods for extracting functional motifs and structure–property relationships of materials from machine learning models is imperative.

The research was published in National Science Review.


Provided by Science China Press