Topological Material Database and Machine Learning on It

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The establishment of topological band theory has made the topological classification of electronic states of solid materials increasingly rich and complete. An effective model based on the energy band inversion reveals its microscopic mechanism. Symmetry analysis of Bloch wave function provides direct and effective tools for identifying the class of topological states, known as the symmetry indicator theory and/or topological quantum chemistry theory. High-throughput electronic structure calculations can screen all known crystal materials and establish a topological materials database, which greatly promotes the discovery of topological materials. But how to turn the physical mechanisms and empirical parameters into intuitive chemical images and material experiences is crucial to exploring and designing new topological materials. Machine learning based on data analysis can discover and establish correlations between different physical quantities, and deepen our understanding of the structure, component and property of materials and their mutual influence. By analyzing tens of thousands of data in the topological materials database through machine learning, quite accurate topological classification of materials can be achieved. The most important features of crystal structure and component valence electrons are found to affect topological classes. These features are closely related to the empirical parameters in the effective model Hamiltonian, which provides guidance for finding and establishing the causal relationship between material chemistry experience and physical mechanism.