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第26回　情報統合型研究交流会

Finding physically meaningful descriptors for high-throughput computational materials design: Methods and applications

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Discovering the best material for a given function (e.g., a catalyst or an electronics component) is a key challenge of our time. Out of billions possible materials, some selected properties of less than 300,000 materials are known to date. With the increase of computational power, high-throughput *ab initio* calculations became a promising way to overcome this challenge. However, a reliable first-principles prediction of complex materials properties (such as surface phase diagrams or turn-over frequency of a catalytic reaction) remains inaccessible. This problem can be addressed by finding descriptive parameters (descriptors) that are much easier to evaluate than a target complex property, but have a strong correlation with the property. In this work, we develop a compressive sensing methodology for finding descriptors from the analysis of computational (and/or experimental) materials data. The methodology allows for assessing the physical meaning of the descriptors and, consequently, their causal relation to the target property. The approach is demonstrated by applications to crystal structure prediction and activation of carbon dioxide at surfaces.

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