第387回触媒科学研究所コロキウム

Patterns, Correlations, and Causality in Big Data of Materials: Analytics for Novel Materials Discovery

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2016年4月25日(月)15:00—16:00

創成科学研究棟4階セミナー室B・C

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Big data of materials are structured in a way that is typically not visible by standard tools. Furthermore, with respect to a certain (desired) property, the "chemical compound space", which contains a practically infinite amount of different materials, is very sparsely populated. Thus, a key issue in data-driven materials science is to find the proper descriptive parameters (descriptors) that identify the materials-property related structures of this huge space.
We will show that and how compressed sensing, originally designed for representing a complex signal in the lowest possible dimensionality, can select, out of a huge-dimensional space of potential descriptors (features), a low-dimensional descriptor. Examples are crystal-structure and stability prediction and the prediction of the band gap of binary and ternary compounds. By applying sensitivity analysis, supervised pattern discovery, and causal inference techniques, we discuss the causal relationship between the selected descriptors and the predicted physical properties. We will also address how the recently establishes NOMAD (novel materials discovery) Laboratory, a European Center of Excellence (http://NOMAD-CoE.eu), will address these issues.

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Dr. rer. nat. in 1978, and Habilitation and venia legendi in 1984 at Technical University Berlin. Scientific staff member of the Physikalisch-Technische-Bundesanstalt, Braunschweig from 1978 to 1987. He was appointed to be the Director at the Fritz Haber Institute of the Max Planck Society in 1988. He is Professor at the Technical University and the Free University in Berlin. Since 2005, he is Distinguished Visiting Professor at the University of California, Santa Barbara. From April, 2016, he is Visiting Professor at the Institute for Catalysis, Hokkaido University. He received many honors and awards; for example, Max Planck Research Award in 2001, Medard W. Welch Medal and Prize in 2003, Max-Born-Medal and Prize in 2004, Ernst Mach Honorary Medal for Merit in the Physical Sciences in 2008, Rudolf Jaeckel Prize in 2010, and a Dr. honoris causa from Lunds University. Author of 542 papers, including 114 papers in Phys. Rev. Letters. Board member of many international organizations.

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