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Utilizing Knowledge on Scientific Principles on Material Properties for Materials R&D

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A material search method without numerical data but with scientific principles has been proposed. It utilizes scientific principles in a form of connections of various materials properties. The connections of properties are made into network-type knowledge database, and a system to search these connections has been developed.

1. Introduction

Recently, data analysis using machine learning techniques, usually called 'materials informatics', has intensively tried to introduce in materials research and development. Machine learning algorithms and programs are already given for free of use, mostly in "python" computer language. Then, the questions are, 1) how to find proper inputs to obtain desirable outputs, 2) what if only few numerical data is available, and so forth.

The author has been developing a material search technique named "materials curation®", which utilize not numerical data but knowledge on scientific principles. In this talk, the basic concept of the technique and examples of knowledge utilization will be explained. Then, the development of a tool for knowledge utilization, network-type knowledge database and search system, will be described.

2. Concept

For machine learning, one needs to input numerical data for the exploration space. In other words, if numerical data on a certain property is not input, that property is out of exploration (see Fig. 1). Therefore, there is huge space unexplored with machine learning. Desired materials are not necessarily inside the exploration space with numerical data.

In order to explore space without numerical data, we use scientific principles, which are established and described in textbooks. Let's give an example of how to use scientific principles. Assume that one only has numerical data on property-A, but knows that property-B is linearly proportional to property-A and property-C is inversely proportional to property-B. Then there are material-X having A-value of 3.0 and material-Y of 5.0. If one needs a material with high value in property-C, which material to choose, X or Y? One can obtain an answer, X, without any numerical data on property-C.

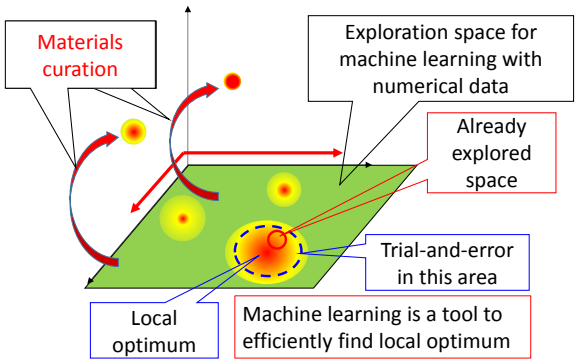

Fig. 1 Schematics of material exploration space in machine learning and materials curation.

The above example is extremely simplified but demonstrates practical usefulness of knowledge on relations among properties, the author believe.

3. Examples

3.1 HOMO-LUMO gap and formation enthalpy

When atom A and atom O bind to make a molecule AO, bonding orbital (HOMO) and anti-bonding orbital (LUMO) are formed. The valence electrons of A atom and O atom both occupy LUMO, then the energy stabilization of bond formation (= formation enthalpy of the molecule) is (α+β) + β as shown in Fig. 2. From the figure, HOMO-LUMO gap energy is also equal to (α+β) + β. This means that the HOMO-LUMO gap is equal to the formation enthalpy of the molecule.

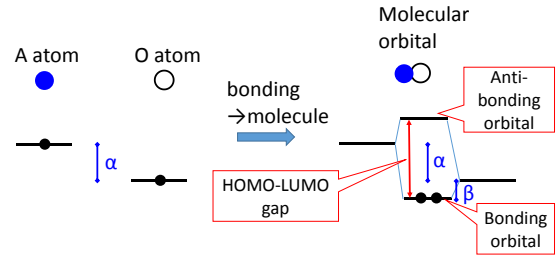

Fig. 2 Energy schematics of molecule formation: HOMO-LUMO gap v.s. formation enthalpy.

3.2 Redox potential and formation enthalpy

Standard redox potential of batteries, E°, is known to be determined by standard Gibbs energy change, ΔG°, with the following relation, $E° = -\Delta G°/nF$ in electrochemistry, where n is a valence and F is Faraday constant (= 9.65×10^4 C/mol).

If there is no gas formation included in the redox reactions, we can approximate ΔG° by ΔH° (formation enthalpy). For silver oxide battery (SR**), redox reaction is: +: $Ag_2O + H_2O + 2e^- \rightarrow 2Ag + 2OH^-$ with 0.342 V, and -: $Zn + 2OH^- \rightarrow ZnO + H_2O + 2e^-$ with -1.260 V, giving E°=1.602 V for total reaction: $Ag_2O + Zn \rightarrow 2Ag + ZnO$. Formation enthalpy of ZnO and Ag_2O are 350.5 and 31.1 kJ/mol, respectively. With n=2, E° is 1.655 V with ΔG° being approximated by ΔH°. This technique has been used to find a transition metal element good for lithium ion batteries by first-principles calculations [1].

4. Database of Scientific Principles

At the recognition of the usefulness of such relations among properties, the construction of a network-type knowledge database on material properties and search system of the network using graph theory has started. Fig. 3 shows the overview of the database and search system. At the moment, the author is collaborating with a company on the development of semi-automatic extraction of scientific principles from texts to speed up data accumulations.

5. References

[1] G. Ceder, M. K. Aydinol, A. F. Kohan, *Computational Materials Science* **8** 161 (1997).

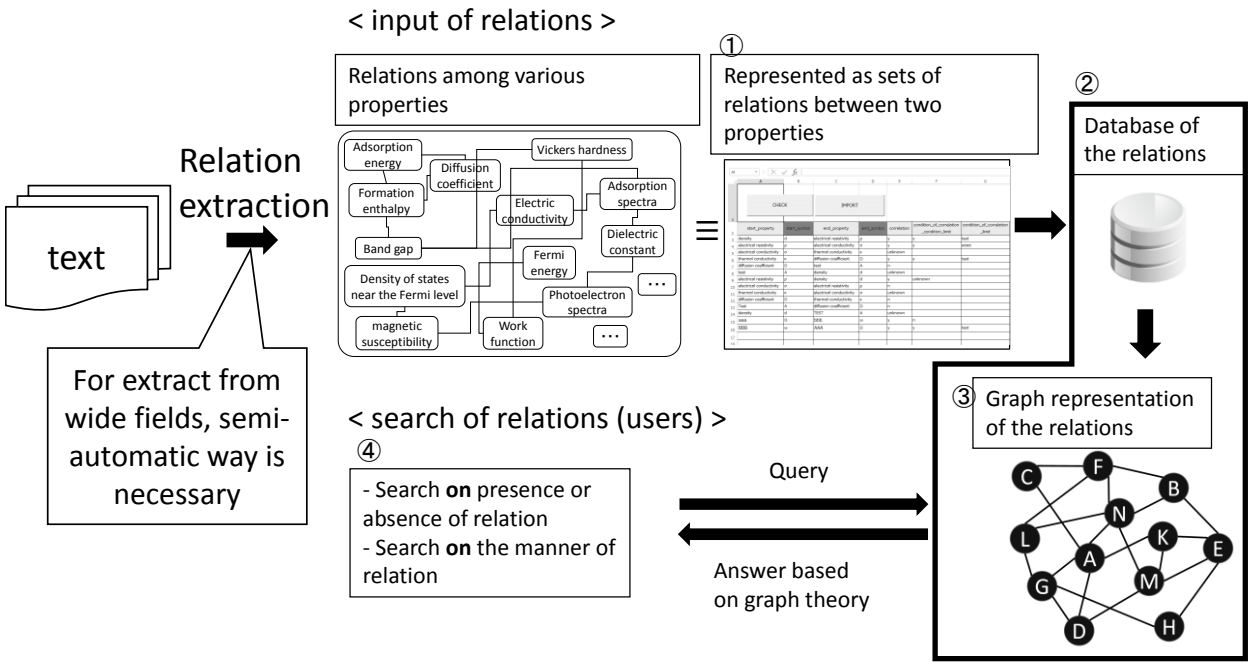

Fig. 3 Schematic illustration of the network-type knowledge database and the searching system of relations among various materials quantities.