Materials fingerprints identified for informatics

Despite the vast amounts of data piling up in established materials databases, there has not been much success in forming quantitative relations between the properties and the overall function of a material. The ability to predict future materials and their properties from the information contained in these repositories is a much sought after goal in materials research. It is then not surprising that this is also a mighty challenge, with few explorers groping in the dark due to a lack of better tools and techniques.

A team of researchers, led by Stefano Curtarolo of Duke University and Alexander Tropsha of The University of North Carolina at Chapel Hill, has now employed a set of novel *materials fingerprints* to quantify a material's physical, electronic, and geometrical properties and to visually map the underlying similarities in the form of a *materials cartogram*. Based on this method, the researchers describe a materials space containing superconducting hotspots, which show a high correlation between the physical proximity of the nodes and the critical temperature of the materials they represent.

At the heart of the work are two numerical arrays of descriptors or fingerprints that encode the electronic structure of a material. B-fingerprints are based on band structure and are symmetry-dependent. D-fingerprints are based on density of states and are symmetry-independent. This enables the use of classical approaches to mine, visualize, and model any set of materials. Materials with similar fingerprints seem to correspond to materials with similar properties. For example, taking GaAs as the reference material, the five materials with most similar fingerprints are GaP, Si, SnP, GeAs, and InTe—all of which are known semiconductor materials. The researchers further used a graph-drawing algorithm to create a map of materials connected by their fingerprint similarities. In their article, which was published in the February 10 issue of *Chemistry of Materials* (DOI: 10.1021/cm503507h; p. 735), researchers demonstrate a B-fingerprint network that shows a clear separation between metals and non-metals. There is also high clustering among subgroups, such as semiconductors and bimetals.

The researchers refer to this approach as visualizing and analyzing materials and their properties as materials cartography. This might aid in the prediction of new materials with a given property by being able to identify similar materials. The researchers illustrate this with a superconductor data map that shows high clustering among high-temperature superconductors, as marked in the figure. Using a custom quantitative materials structure–property relationship (QMSPR), they were able to predict—with over 94% accuracy—whether the critical temperature of a given material would fall above or below a threshold temperature. This is interesting, as the fingerprints by themselves do not contain any information other than the material's electronic structure.

"The challenge that we face today is to translate data into knowledge by establishing relationships between inherent material structural properties and their function," Curtarolo and Tropsha said in a communication. "Our studies help bridge this gap, enhancing our ability to explore and exploit these data for rational design of novel materials with the desired function."

Databases such as AFLOWLIB and ICSD provided the data used to create the fingerprints. The data for superconductors were taken from the *Handbook of Superconductivity, CRC Handbook of Chemistry and Physics*, and the Supercon database.

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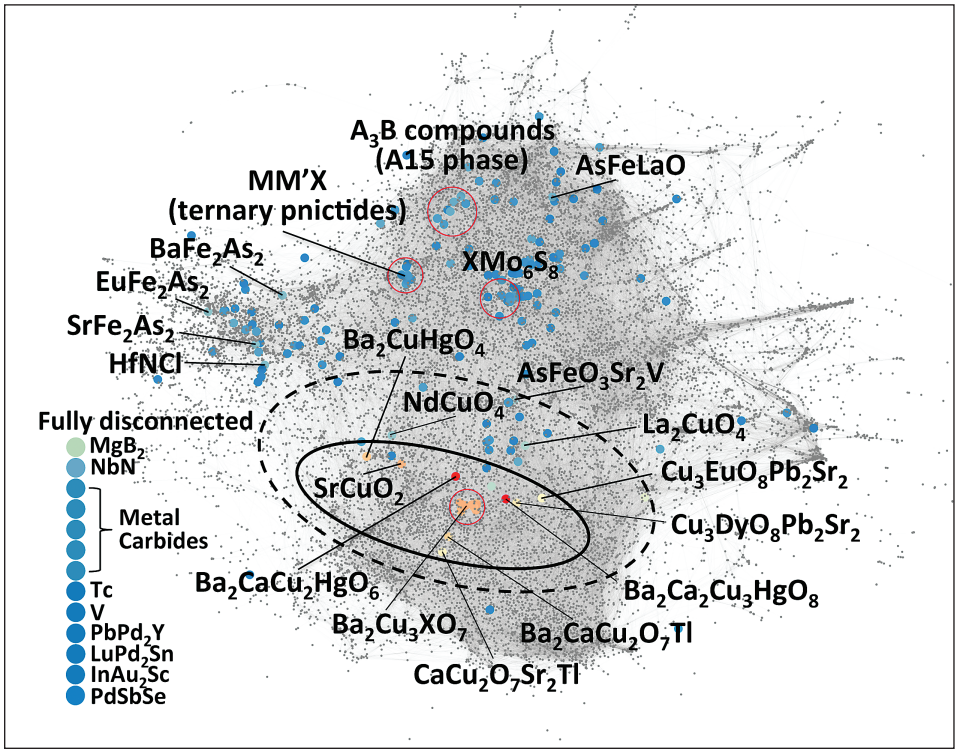

Materials cartography: Mapping the superconductivity critical temperature with relevant regions outlined. Reproduced with permission from *Chem. Mater.* **27** (3) (2015), DOI: 10.1021/cm503507h; p. 735. © 2014 American Chemical Society.

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