Designing Single Molecule Magnet with Data Mining

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Quantum calculation plays a very important role in the process of materials design nowadays. For a material with a given hypothesized structural model, the electronic structure, as well as many other physical properties can be predicted by a series of optimizing processes. The task of materials design is to make the correlations between the features of an optimal structure model of materials, as well as its derived physical properties clear and to determine a strategy to modify the materials to obtain desired properties. However, such correlations are usually hidden and difficult to uncover or predict by experiments or experience. As a consequence, the design process is currently performed through time-consuming and repetitive experimentation and characterization loops, and to shorten the design process is clearly a big target in materials science.

In an effort to improve on existing techniques, we propose a first principle calculation-based data mining method and demonstrate its potential for a set of computationally designed single molecular magnets with distorted cubane $Mn^{4+}Mn^{3+}$ core. In our method, we use advanced statistical mining algorithms, in particular multiple linear regression with LASSO regularized least squares [1] to solve the sparse approximation problem on the space of structural and physical properties of materials. The conditional relations of each feature on to all the other features are evaluated in terms of prediction [2]. Based on the obtained relations, a graph representing relations between all properties of materials can be constructed and optimized (Fig. 1). The obtained graph is not only significant for the comprehension of the physics relating to the materials, but also valuable for the guidance of effective material design [3].

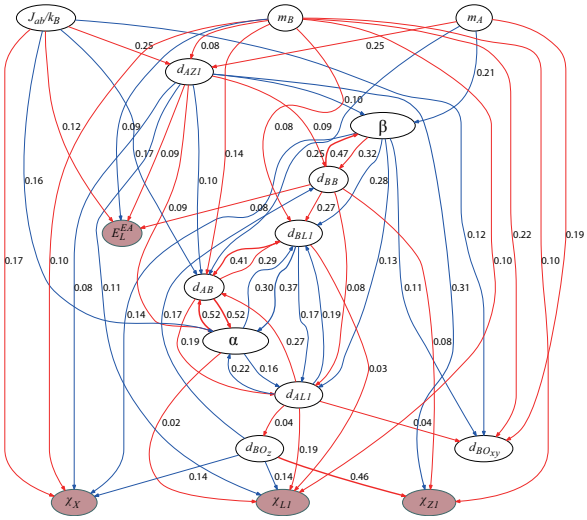

Fig. 1 The graph represents all relations between the features of the designed SMMs

References:
1) R. Tibshirani, J. R. Statist. Soc. B 58, 267 (1996).
2) B. Efron, T. Hastie, I. Johnstone, and R. Tibshirani, Annals of Statistics 32, 409 (2004)
3) C. H. Dam et al., J. Chem. Phys. 140, 044101 (2014)
Keywords: Data mining, magnetic materials, Density functional theory
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