Integration of Data Mining and Structure Analysis for Materials Design

DAM Hieu-Chi（Japan Adv. Inst. of Sci. and Tech, Associate Professor)

（FY2017-2020）

Brief overview

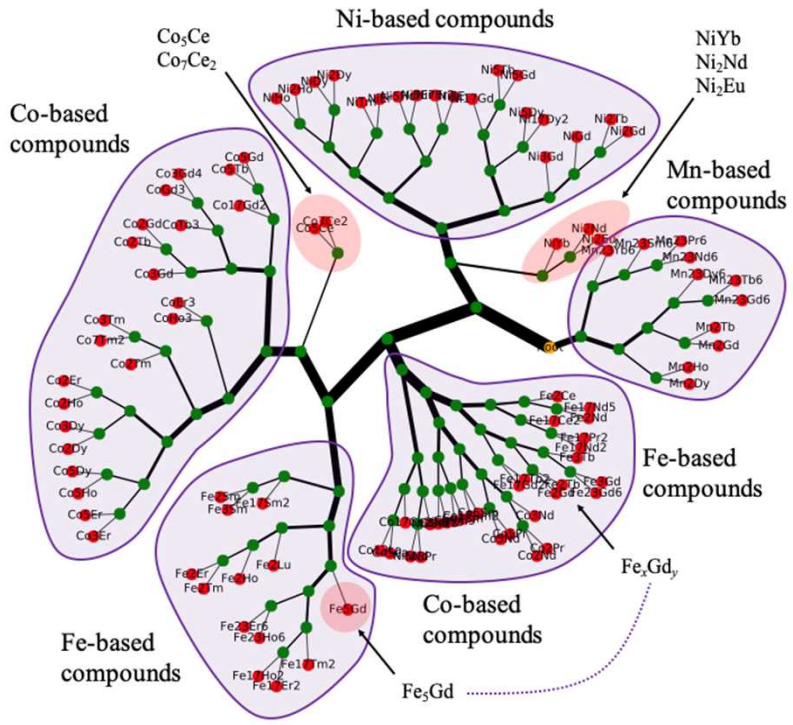
In this research, I focus on the development of AI methods to support human comprehension and creativity, and a mechanism by which humans can intervene in the process of discovering novel materials and physical phenomena. My research concentrates on revealing the mechanism underlying magnetic properties, in parallel with the design of new crystalline magnetic materials by integrating computational materials science, advanced data science, and structure analysis techniques. I also aim at developing a basis for interdisciplinary experimental, computational, and data-driven approaches, and explainable AI that will help researchers drive progress and discovery in materials science, in order to understand physicochemical phenomena.

I actively consider three fundamental issues: materials representation, measure for similarity between materials, and acquiring scientific knowledge on materials from data.

Achievement

1. Development of interpretable generic material descriptors: We have developed the Orbital Field Matrix (OFM) [1, 2], that can express the structure and properties of complex materials with various elements by incorporating atomic orbital and crystal field information.
2. Materials similarity measure with respect to physical properties: We have developed a regression-based measure that can determine the similarity between materials with respect to a specific physical property [3]
3. Scheme for interpreting the output of sophisticated data-driven approaches: We identified a robust and straightforward scheme for interpreting the output of a sophisticated data-driven approach that predicts the Curie temperature of a binary alloy consisting of transition metals and rare-earth elements [4].

Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）



Hierarchical cluster structure of rare-earth transition alloys utilizing information from the similarity measure with respect to the Curie temperature of ferromagnets.

Reference/Link

[1] T. L. Pham and *H. C. Dam *et al.*, STAM, 18, 1, 756-765 (2017).
[2] T. L. Pham and *H. C. Dam *et al.*, J. Chem. Phys., 148, 20, 204106 (2018).
[3] D. N. Nguyen and *H. C. Dam *et al.*, IUCrJ, 5, 6, 830-840 (2018).
[4] H. C. Dam and H. Kino *et al.*, J. Phys. Soc. Jpn., 87, 113801 (2018).