データ科学手法による磁性材料探索

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Data-Science Approach to Magnetic Materials Exploration

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Data-science approaches with rapidly growing data have recently brought a new trend of research and development to a variety of fields in science and technology. In materials science, it is now widely called ”Materials Informatics (MI)”, as often seen in several related world-wide projects[1–5]. The key strategy is to integrate data-science techniques with experimental, theoretical, and computational ones. Especially big data generated by computational simulations together with existing experimental databases are the target of data-science methods such as data mining and machine learning interleaved with appropriate physical modeling and descriptors. In MI, first-principles density-functional-theory calculations among the computational approaches play an important role for supplying data and knowledge on materials complemental to the experimental databases. This is one of the characteristic features of MI contrast to the preceding ”Bioinformatics”. In this talk, I shall introduce some fundamental issues of the data-science approaches to the exploration of magnetic materials in our research project MI^2I.

References

1) Materials Genome Initialtive (MGI): https://www.whitehouse.gov/mgi
2) Materials Design at the Exascale (MAX): http://www.max-center.eu
3) Novel Materials Discovery (NOMAD): http://nomad-coe.eu
4) An e-infrastructure for software, training, and consultancy in simulation and modeling: http://cordis.europa.eu/project/ rcn/198333_en.html
5) Materials Research by Information Integration Initiative (MI^2I): http://www.nims.go.jp/eng/research/MII-I/index.html