Computational exploration of new permanent magnet compounds

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I will discuss current status and challenges for permanent magnet research by information integration. Strong magnet compounds such as $Nd_2Fe_{14}B$, $Sm_2Fe_{17}N_3$ and $NdFe_{12}N$ consist of three elements, namely rare-earth, iron and the third element. A natural question is: What is the best third element, and what about the fourth in a quaternary compound? This is an issue to be tackled by computational screening. As an example, we will present first-principles calculations of $ThMn_{12}$ type iron-based compounds. However, brute-force search based on first-principles calculations is computationally demanding even if using supercomputer facilities, since the number of combinations of chemical composition increases rapidly as the number of elements in a compound is increased. Machine learning is a possible solution to improve the efficiency drastically. It is found that Gaussian process regression using 7 descriptors accurately reproduces the Curie temperatures of bimetal alloys composed of transition-metal and rare-earth elements. This technique can be utilized for virtual screening. Another issue is exploration of crystal structure. Saturation magnetization is expected to be larger as the iron content increases. Hence, the crystal structure of new iron-rich phases is of particular interest. Crystal structure prediction is a hot topic in computational materials science in the past decade, and various efficient algorithms have been developed. Recent progress and applications will be reviewed.