Multi-objective virtual screening with structure prompting

[*]Duong-Nguyen NGUYEN[1], Minh-Quyet HA[1], Hiori KINO[2], Takahashi MIYAKE[3], Hieu-Chi DAM[1, 4]

[1] *Japan Advanced Institute of Science and Technology, Nomi, Ishikawa, Japan*

[2] *National Institute for Materials Science, Tsukuba, Ibaraki, Japan*

[3] *National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki, Japan*

[4] *International Center for Synchrotron Radiation Innovation Smart, Tohoku University, Sendai, Miyagi, Japan*

[*]nguyennd@jaist.ac.jp, dam@jaist.ac.jp

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We introduce a structure prompting (SP) program to accelerate multi-objective evolutionary search of materials. Focusing on the discovery of outstanding Sm-Fe magnets, the SP system aids in the search for new main-phase crystals that maximize symmetrical information, stability, and saturated magnetization while minimizing the formation of potential sub-phase crystals. The framework leverages the Dempster–Shafer theory to recommend *micro scale-prompt* constructed based on chemical composition and crystal symmetry with a high potential stability. During the genetic-algorithm structure search for optimal skeleton structures that match with *micro scale-prompt*, we introduce *atomic scale-prompt* structure generator with two symmetry-based transformation operators to stimulate and accelerate the evolutionary process. Finally, high-potential skeletons are validated for physical properties using first-principle calculations. In experiments on Sm-Fe-based crystals, the proposed SP system not only accelerates but also extends solutions obtained using the conventional universal structure predictor: Evolutionary Xtallography genetic algorithm. Moreover, it facilitates the elucidation of high-symmetry meta-stable structures by establishing correlations among formation energy, saturated magnetization, and geometric parameters, which encompass atomic density, inter-atomic distance distribution, and crystal symmetry. A reverse stability order of optimal skeletons in the $SmFe_{12}$, $SmFe_5$, and $SmFe_2$ phases was observed at higher external pressures, which may be attributed to shifts in interatomic distance distribution. The trigonal and tetragonal crystal systems of the $SmFe_{12}X_{1:5}$ compounds exhibited competing stabilities, with X representing N, B, and C. This study not only advances our fundamental understanding of geometrical stability mechanisms but also presents a robust framework applicable to a wide array of materials, opening new avenues for tailored material design and discovery.

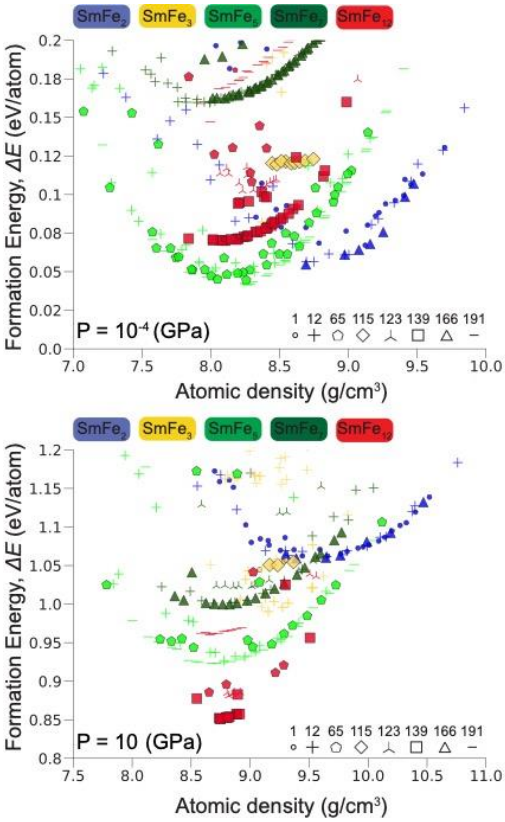

Figure 1: Formation energy and atomic density of screened $SmFe_k$ k = {2, 3, 5, 7, 12} structures using structure prompting program.

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