Research Title Development of methods for predicting physical properties using machine-learning techniques

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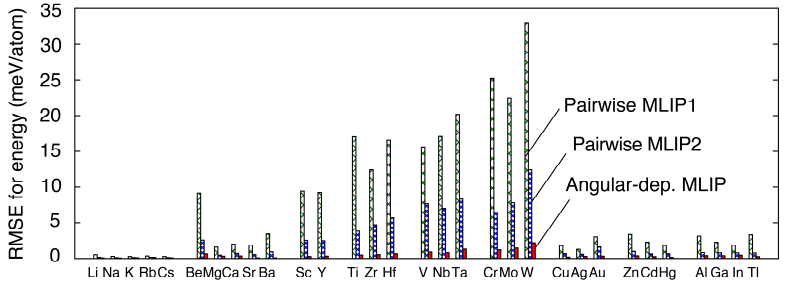
Research Area : Advanced Materials Informatics through Comprehensive Integration among Theoretical, Experimental, Computational and Data-Centric Sciences（PO：Shinji Tsuneyuki）

Brief overview

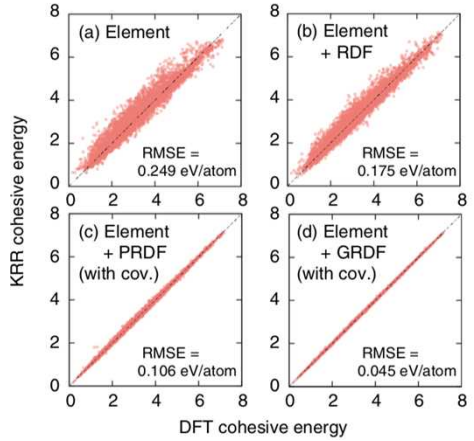
Descriptors play a crucial role in the construction of machine-learning prediction models of physical properties aimed at accelerating materials design. In this study, simple descriptors for crystal structure that are applicable to a wide range of physical properties will be developed. I will dedicate myself to proposing first-principles machine-learning interatomic potentials of a wide range of materials and constructing prediction models of first-principles physical properties.

Achievement

The representations of a compound, called “descriptors” or “features”, play an essential role in constructing a machine-learning model of its physical properties. In this study, we adopt a procedure for generating a set of descriptors from simple elemental and structural representations. They exhibit good predictive performances.



Machine learning interatomic potential



Comparison of cohesive energy calculated by DFT calculation and that calculated by the KRR prediction model.

Reference/Link

https://www.jst.go.jp/kisoken/presto/en/research_area/ongoing/areah27-4.html