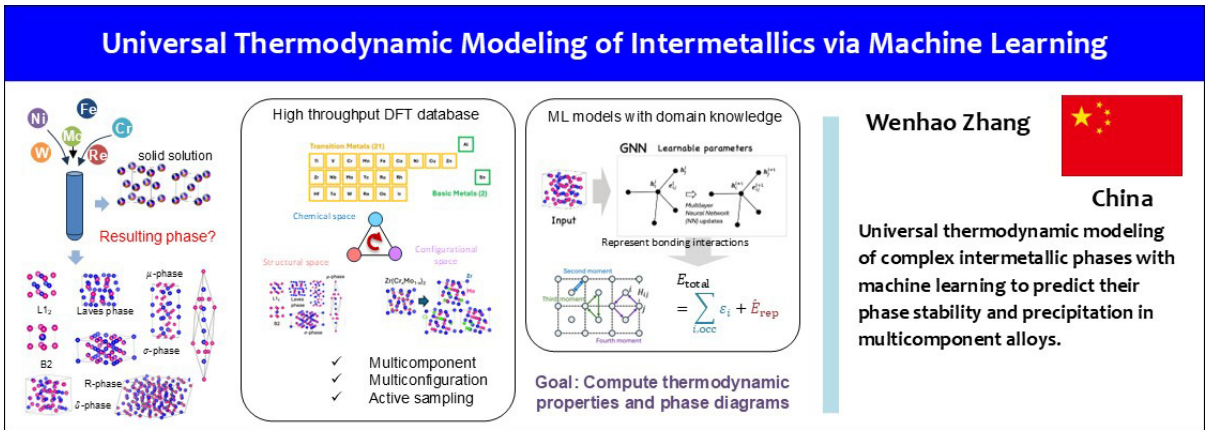
Universal Thermodynamic Modeling of Intermetallics via Machine Learning

ICYS Research Fellow Dr. Wenhao Zhang



■Research

Phase diagrams—the maps from chemical composition, temperature, and pressure to the specific arrangement of atoms—are both scientifically interesting and practically very important. At the scientific level, it is always fascinating, but difficult, to understand how atoms self-arrange into different crystal structures; and practically, materials' properties—mechanical, thermodynamic, and electrical—are all macroscopic consequences of these self-arrangements of atoms. To predict phase diagrams, an accurate potential energy surface that covers all kinds of atomic arrangements is needed. Recently, machine learning models, such as graph neural networks, have emerged as powerful tools that allow us to sample such potential energy surfaces rapidly. While these models are highly successful, they are not physically transparent and require large amounts of data to train. Focusing on metallic and intermetallic phases, my research at ICYS aims to integrate domain knowledge of electronic structure into machine learning models so that the energy of bond formation between atoms can be explicitly modelled and transparently examined. Using such models, I seek not only to predict the stability of materials and structures, but also their possible functional properties.

■Comments

ICYS provides me the opportunity to work independently. This independence allows me to pursue my own research topics driven by my insights and curiosity, in a well-supported environment provided by ICYS and NIMS. For a young researcher like me, this independence also means responsibility—the responsibility to set research directions, to keep learning and to focus on research. Because of this, I believe ICYS will prepare me to become a researcher who can stand on his own two feet.

■Link

https://www.nims.go.jp/icys/research/#ZHANG