Computational Materials System Design by Phases Research Lab

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The Phases Research Lab (PRL), led by Prof. Zi-Kui Liu, is focusing on computational thermodynamics and kinetics in terms of the CALPHAD approach, first-principles calculations based on density functional theory, and machine learning, together with their integration for understanding defects, phase stability, and phase transformations, and designing and tailoring materials processing and properties. Recently Prof. Liu and the members at PRL developed the zentropy theory that can predict macroscopic functionalities including singularity from quantum mechanics and statistical mechanics based solely on density functional theory; and derived the general flux equations and predicted the cross-phenomenon coefficients from the combined law of thermodynamics. Currently, the PRL is financially supported by both federal funding agencies including the Department of Energy (DOE), Department of Defense (DOD), and National Science Foundation (NSF), and industrial companies, e.g., tech Inc. The ongoing projects at PRL include, for example, the design and manufacturing of ultrahigh temperature refractory alloys supported by DOE, zentropy theory for transformative functionalities of magnetic and superconducting materials supported by DOE, a molten salt community framework for predictive modeling of critical characteristics supported by DOE, functionally graded metallic materials by directed energy deposition additive manufacturing: computational design, fabrication and validation supported by NSF, development of a new open-source ecosystem for materials science supported by NSF, and design and fabrication of additively manufactured functionally graded materials by DOD.