Demonstration of a fresh computer program for phase diagram calculations

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Abstract

Our motivation in developing this indigenous software is to create a versatile tool for the calculation and optimization of phase diagrams. Beyond this, we envision seamless integration with diffusion studies [1] and phase-field simulations [2] to enhance practical applicability. While existing software packages such as Lukas, ChemSage, MatCalc, ThermoCalc, Pandat, MTDATA, CaTCalc, FactSage, PyCalphad, and OpenCalphad, have made substantial contributions to phase diagram calculations [3], our initiative uniquely addresses specific needs and challenges, providing a fresh perspective on the application of computational thermodynamics.

In the realm of computational thermodynamics, we are at the forefront of introducing a new Python software package specifically designed for calculating phase diagrams. Figure 1 displays the initial logo of our software program.

This workshop stands as a vital platform, offering participants a thorough grasp of computational thermodynamic software with a prime focus on the CALPHAD method. It explores the intricacies of different software functions, covering routines for reading thermodynamic databases and conducting binary phase diagram calculations. Moreover, our software produces results in a format that allows easy integration into diverse tools and workflows, ensuring flexibility for seamless incorporation into existing computational frameworks.

Our software transcends being a mere standalone tool; it represents a broader vision advancing the comprehension and application of computational thermodynamics. Its creation is in harmony with the escalating need for sophisticated and user-friendly tools in materials science and metallurgy. This initiative lays the groundwork for future advancements, including integration with diffusion studies and phase-field simulations, opening new avenues for researchers, and enriching the exploration of phase diagram intricacies.

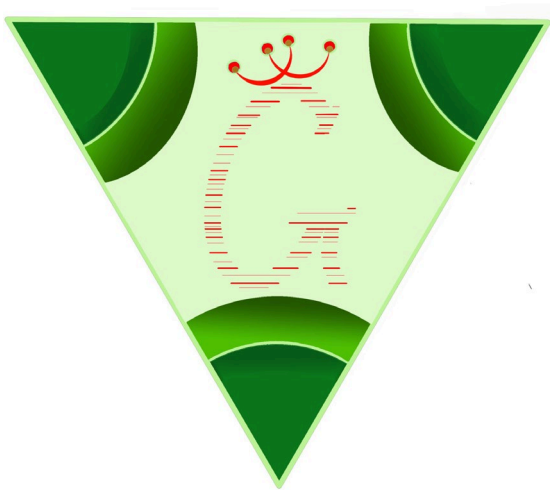

Figure 1. Logo for our phase diagram calculation software

References

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[3] Taibai Fu, et al. "A new algorithm to calculate binary phase diagrams,", *Comput. Mater. Sci.,* 159 (2019): 478

Biographical Note

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