Thermodynamic Understanding and Prediction of Critical Phenomena in Solids

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Thermodynamics of critical phenomena in a system is well understood in terms of the divergence of molar quantities with respect to their respective conjugate potentials[1]. However, the prediction and the microscopic mechanisms of critical points and the associated property anomaly, i.e. divergence of molar quantities, remain elusive. In this presentation, our recent progress will be discussed. It is shown that while the critical point is typically considered to represent the limit of stability of a homogeneous system when the system is approached from a homogenous state to the critical point, it denotes the mixture of several homogeneous subsystems to become a macro-homogeneous system when the critical point is approached from a heterogeneous system. By systematically sampling important homogeneous subsystems or states, it is demonstrated that the statistical mixture of these states can predict the critical points and the associated property anomaly[2]. Furthermore, a general thermodynamic framework of critical phenomena will be discussed[1].

References:

[1.] Liu, Z. K. & Wang, Y. Computational Thermodynamics of Materials. (Cambridge University Press, 2016).

[2.] Liu, Z. K., Wang, Y. & Shang, S. L. Thermal Expansion Anomaly Regulated by Entropy. Sci. Rep.4,7043 (2014).