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Thermodynamics beyond Equilibrium and its Application to Diffusion

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Thermodynamics is a science concerning the states of a system whether it is stable, metastable, unstable or any states between ¹, far beyond the equilibrium states only believed by some . In this presentation, the thermodynamic fundamentals are reviewed and discussed in terms of theory, modeling, and applications along with the impact of first-principles calculations based on the density functional theory ². Our recent activities on thermodynamic instability and the associated extraordinary physical properties are presented, including the 100 year old mystery of INVAR effects ³. Furthermore, the prediction of diffusivity in solid phases based on thermodynamic energetics is discussed ^{4,5}.

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