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this book compiles selected publications authored or co authored by the editor to present a comprehensive understanding of following topics 1 density functional theory and calphad modeling 2 computational tools and 3 applications of computational thermodynamics it is noted that while entropy at one scale is well represented by standard statistical mechanics in terms of probability of individual configurations at that scale the theory capable of counting total entropy of a system from different scales is lacking the zentropy theory provides a nested form for configurational

entropy enabling multiscale modeling to account for disorder and fluctuations from the electronic scale based on quantum mechanics to the experimental scale based on statistical mechanics using free energies of individual configurations rather than their total energies in standard statistical mechanics the predictions from the zentropy theory demonstrate remarkable agreements with experimental observations for magnetic transitions and associated emergent behaviors of strongly correlated metals and oxides including singularity and instability at critical points and positive and negative thermal expansions without the need of additional truncated models and fitting model parameters beyond density function theory this paves the way to provide the predicted phase equilibrium data for high throughput predictive calphad modeling of complex material systems and those individual configurations may thus be considered as the genomic building blocks of individual phases in the spirit of materials genome

includes entries for maps and atlases

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