



INTERDISCIPLINARY CENTRE FOR  
ADVANCED MATERIALS SIMULATION

## ICAMS Special Seminar

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### Entropy

Entropy is a key quantity in science, particularly thermodynamics. Its definitions in terms of classic thermodynamics and statistic mechanics are well established. The Boltzmann formula  $S=k_B \ln w$ , with  $k_B$  and  $w$  being the Boltzmann constant and the number of microstates, gives the logarithmic connection between entropy and probability. The fundamental concept in this formula is that each microstate has the same probability to be observed statistically. A more general formula is written as  $S=-k_B \sum p_i \ln p_i$ , with  $p_i$  denoting the probability for the microstate  $i$  being observed statistically, also known as Gibbs entropy. The significance of this general formula with respect to the Boltzmann formula resides on the dependence of  $p_i$  on temperature, pressure, electric and magnetic fields, which results in anomalies in a macroscopically homogeneous system when new metastable microstates are introduced. In this presentation, some examples are discussed such as thermal expansion behaviors of Invar/anti-invar alloys and water/ice.