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Nota di bibliografia	Includes bibliographical references at the end of each chapters.
Nota di contenuto	Introduction -- A Primer in Probability -- Phase Space Probability Distributions for Various External Conditions -- Relating Probability Density Functions to the Behaviour of Systems -- The Strategy of Nested Sampling -- Nested Sampling for Materials -- Equations of State -- Parallelising Nested Sampling -- Hamiltonian Monte Carlo for the Canonical Distribution -- Hamiltonian Monte Carlo for Nested Sampling -- Conclusion of Thesis and Further Work.
Sommario/riassunto	This thesis develops a nested sampling algorithm into a black box tool for directly calculating the partition function, and thus the complete phase diagram of a material, from the interatomic potential energy function. It represents a significant step forward in our ability to accurately describe the finite temperature properties of materials. In principle, the macroscopic phases of matter are related to the microscopic interactions of atoms by statistical mechanics and the

partition function. In practice, direct calculation of the partition function has proved infeasible for realistic models of atomic interactions, even with modern atomistic simulation methods. The thesis also shows how the output of nested sampling calculations can be processed to calculate the complete PVT (pressure–volume–temperature) equation of state for a material, and applies the nested sampling algorithm to calculate the pressure–temperature phase diagrams of aluminium and a model binary alloy.