Abstract Submitted
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The Density of States: Counting that Counts GREGORY BROWN, Florida State University / Oak Ridge National Laboratory — Wang-Landau method and associated Multicanonical Monte Carlo methods make it possible to calculate the density of states g(E) for thermodynamic systems. This is particularly useful for first-principles calculations, where temperature-dependent quantities like the specific heat and susceptibility can be calculated from, say, 50000 configurations. We have successfully employed an approach combining the classical Heisenberg model of magnetism with first-principles LSMS computations to calculate Tc in transition metal alloys. The thermodynamic properties of the system can be calculated directly from the ln[g(E)] and its derivatives.

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