

Abstract Submitted
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A Finite Temperature First-Principles Model for Spin Fluctuations YI WANG, SHUNLI SHANG, LONG-QING CHEN, ZI-KUI LIU — In the past decades, the steady increasing in both computer power and the efficiency of computational methods has made it realistic the accurate first-principles calculations of material properties at finite temperature. The current frontier is how to extend the first-principles approach when it becomes important of the role of the internal degrees of freedom, which is beyond the spatial degrees of freedom of a material. One of important examples is the interplay between magnetic and lattice fluctuations at finite temperature. Solution of this enigma can reveal the microscopic origin of the novel properties of many materials. Hereby we propose a general framework to calculate the Helmholtz energy for system with spin fluctuations. The theory has been applied for EuTiO₃. The energetics includes 256 spin configurations, of a 2x2x2 supercell, which are reduced to 14 not equivalent ones. We find a Schottky anomaly in the specific heat at $T = 5.8$ K which is matching closely to the Neel Temperature of 5.5 K for EuTiO₃.

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