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Landau Theory of Trifluoride Negative Thermal Expansion Materials[1] GIAN GUZMAN-VERRI, U of Costa Rica and Argonne Natl Lab, RICHARD BRIERLEY, Yale University, PETER LITTLEWOOD, Argonne Natl Lab and U of Chicago — Negative thermal expansion (NTE) is a desirable property in designing materials that are dimensionally stable and resistant to thermal shocks. Transition metal trifluorides (MF_3, M=Al, Cr, Fe, Ga, In, Ti, V) are a class of materials with ReO_3 structure that exhibit large, isotropic, and tunable NTE over a wide temperature range, which makes them attractive material candidates. They exhibit large coefficients of thermal expansion near their cubic-to-rhombohedral structural phase change, which can be thermally or pressure induced. Though they have recently been the subject of intense experimental research, little work has been done on the theory side and it has almost exclusively focused on zero temperature properties. In this talk, we construct a simple Landau theory of trifluorides and use it to calculate the temperature dependence of the elastic constants, soft phonon frequencies, and volume expansion near their structural transition. We compare our results to existing experimental data on trifluorides.

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