Abstract Submitted
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Thallium-doped $BaFe_2As_2$ crystals: The unusual competition between magneto-elastic coupling and charge doping[1] ATHENA SEFAT, LI LI, HUIBO CAO, BRIAN SALES, MICHAEL MCGUIRE, RADU CUSTELCEAN, DAVID PARKER, Oak Ridge National Lab — We partially substitute thallium for barium and report the effects of interlayer coupling in $Ba_{1-x}Tl_xFe_2As_2$ crystals. We demonstrate the unusual competition between magneto-elastic coupling and charge doping in an iron-arsenide material, whereby T_N temperature rises in $BaFe_2As_2$, and then falls with additional Tl-doping. Evidence from temperature-dependent bulk thermodynamic and transport properties, and neutron diffraction results will be presented. Using LDA, we illustrate that small changes related to $3d$ transition-metal state can have profound effects on magnetism.

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