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Giant pressure-induced volume collapse in the pyrite mineral MnS2

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Dramatic volume collapses under pressure are fundamental to geochemistry. In transition metal materials, collapses are usually driven by so-called 'spin state' transitions- the interplay between the single-ion crystal field and the size of the magnetic moment. Here we show [1] that the classical S= 5/2 mineral Hauerite (MnS2) undergoes an unprecedented (ca. 22 %) volume collapse driven by a conceptually new magnetic mechanism. Using synchrotron x-ray diffraction, we show that cold compression induces the formation of a disordered intermediate. However, using an evolutionary algorithm we predict a new structure with edge-sharing chains is stable. This is confirmed as the thermodynamic ground state by in-situ laser heating. We show that magnetism is globally absent in the new phase, as the low-spin quantum S=1/2 moments are quenched by dimerisation. Our results show how the emergence of metal-metal bonding can stabilise giant spin-lattice coupling in Earth's minerals.

[1] *SAJ Kimber et al, to appear in PNAS (2014)*

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