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Geometrical frustration and macroscopic residual entropy in an elemental boron explained by a frustrated Ising model T. OGITSU, LLNL, F. GYGI, UC Davis, J. REED, LLNL, M. UDAGAWA, Y. MOTOME, U Tokyo, E. SCHWEGLER, LLNL, G. GALLI, UC Davis — An elemental solid, β-rhombohedral boron, is known to have a macroscopic amount (roughly 4 atomic percent) of intrinsic defects, and recent first principles studies have shown that β-boron has *negative defect formation energy* due to the interplay between electron deficiency and the peculiar bonding properties of boron. Consequently, β-boron was shown to be the thermodynamically stable phase at all temperature below melting temperature at ambient pressure over all the other allotropes and polymorphs considered so far. In this talk, we will show that boron defects possesses geometrical frustration that is well described by an AF Ising model on an expanded kagome lattice, and that the model has an exactly degenerate and disordered ground state with macroscopic residual entropy. We will discuss how the peculiar transport properties of β-boron, reported over the past forty years, can be explained by the hopping of boron atoms between the macroscopic amount of degenerate configurations. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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