

Engineering magnetic frustration with impurities

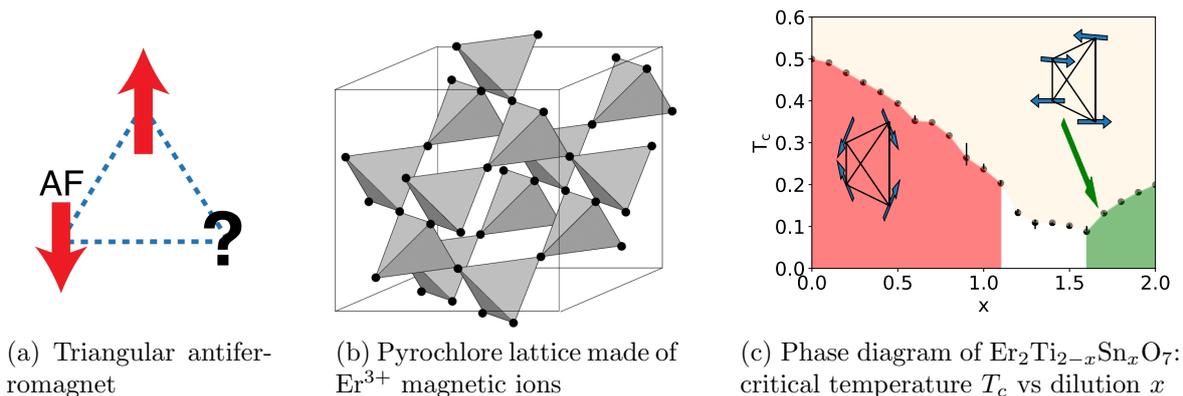
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Sometimes, a little bit of frustration makes life interesting. Although controversial, this statement is certainly correct in physics, where frustration has opened an entire field of research with materials of exotic properties. Frustration refers to the presence of competing forces that cannot be simultaneously satisfied. Frustrated magnets often order in unconventional ways, or do not order at all, even at the lowest temperatures. In this context it is usually believed that pristine crystals are necessary, and impurities are unwanted perturbations.

Our motivation is to take the opposing view, and use impurities as a tool to engineer the properties of frustrated magnets. Motivated by recent experiments on the rare-earth pyrochlore oxide $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$ [1] [Fig. (b)], the idea is to tune the Hamiltonian of our system via non-magnetic dilution x . In other words, to use impurities as a knob to explore unknown parts of the phase diagram. Interestingly, this approach brings us at the frontier between (geometric) frustration and spin glasses. We report the phase diagram of $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$ for $0 \leq x \leq 2$, using classical Monte Carlo simulations. Our calculations reproduce the shape of the experimental phase diagram [1], with a competition between two different types of antiferromagnetic orders, the red and green phases in Fig. (c), and a pronounced asymmetry in favour of the former. We explain the origin of this asymmetry and find that this competition induces an intermediate spin glass phase (in white) where magnetic order disappears. To build a detailed theory, we extract from simulations the specific heat, susceptibility, neutron-scattering structure factor, microscopic fluctuations and spin dynamics.



Keywords— condensed matter, statistical physics, magnetic frustration, spin glass

[1] M. Shirai, R. S. Freitas, J. Lago, S. T. Bramwell, C. Ritter, and I. Zivkovic, “Doping-induced quantum crossover in $\text{Er}_2\text{Ti}_{2-x}\text{Sn}_x\text{O}_7$ ” *Physical Review B*, **96**, 180411 (2017).