Tuesday, Sep 21st at 3:30 pm

(Zoom colloquia: Please find the meeting information below)

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Elastic entropic effects in complex functional matter

The interplay between various degrees of freedom that gives rise to unexpected collective behaviour is a hallmark of complex functional matter. The competition and cooperation between ground states that are energetically close not only generates rich morphologies and phase diagrams, but can also result in an extreme sensitivity to external stimuli, affecting the structural, electronic, magnetic and orbital properties which could be harnessed for practical applications. A crucial aspect of our understanding of complex materials is that the lattice provides an elastic template on which other degrees of freedom such as spin, dipole, orbital and charge couple. At zero Kelvin, state-of-the-art first-principles calculations can make good estimates of the local energy containing implicitly such couplings on a unit cell as well as band structure energy and Coulomb correlations. However, that success does not translate into the ability to describe the highly disordered structures that typically occur in functional materials at finite-temperatures nor to calculate their properties. In this talk, we propose that what has been missing is the correct understanding of the non-trivial and surprisingly subtle effects from anisotropic long range elastic interactions mediated between the local degrees of freedom, which can produce enormous entropic contributions to the free energy that are missed by conventional theories. We illustrate this idea in two classes of materials: the colossal magnetoresistance manganites and the IV–VI chalcogenides. If time permits, I'll discuss how this might be relevant for heat pumps based on solid-state working substances.