Modelling the compositional variation of the properties of magnetic solid state cooling materials.

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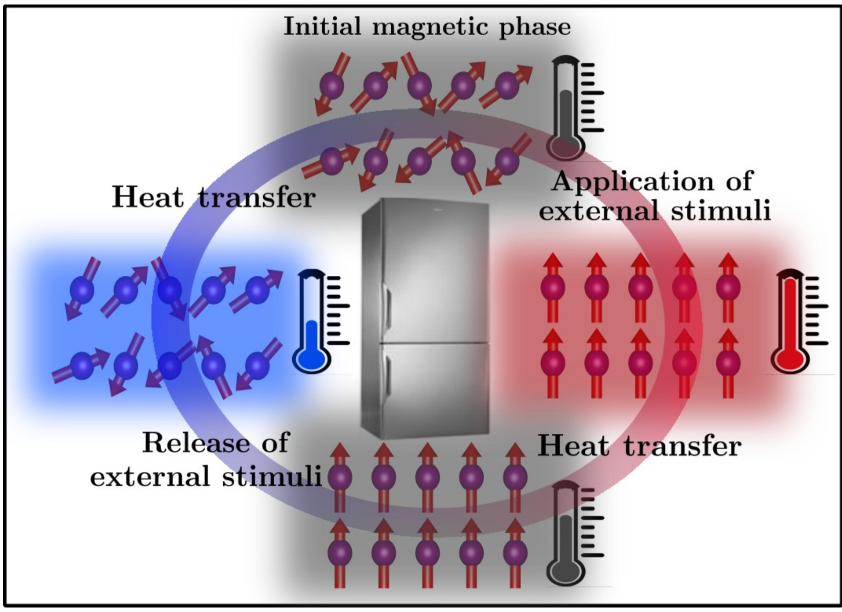

The project: Modern cooling is based almost entirely on a compression/expansion refrigeration cycle - a technology more or less unchanged since its invention over a century ago. It is a high-energy demand mechanism. Yet, it is now close to its fundamental performance limit which is well below what is thermodynamically possible. Recently refrigeration using magnetic materials has emerged as promising for a new and environmentally friendly solid state cooling technology, much more energy efficient and spanning a broad temperature range around 0° C. Randomly oriented magnetic moments align when an external stimulus such as a magnetic field is applied making the solid warm up. By removing this heat using a heat transfer fluid, like water or air, and then removing the stimulus allows the magnetic material to lower its temperature. The heat from the object being cooled is then extracted with the heat transfer fluid and the cycle completed. The changes in entropy and temperature that happen when a field is applied describe a caloric effect. They can be further enhanced, if the mechanism is coupled to a structural transformation. In this project we will use a computational approach that models the material at the sub-nanoscale, where the behaviour of the many interacting electrons is carefully accounted for, to produce interactions among the magnetic moments. A statistical mechanical treatment describes the cooling properties quantitatively. This project will investigate the effect of compositional heterogeneities and disorder on the changes of magnetic and structural state of a material, i.e. phase transitions, where the caloric effects are largest. Starting with superlattices, it will develop a model of the impact of interfaces between regions of different compositions. We will study compositional variation broadening of first order transitions and how to nanostructure a large caloric effect over a prescribed temperature range.

Connection with HetSys CDT: The PhD project will involve a model with degrees of freedom (the magnetic moments or spins) which condense out from the septillions of interacting electrons in a material and study how the interactions among the spins and the phase transitions in their order are affected by compositional uncertainty, nanostructuring and the presence of interfaces. The project combines physics and materials science theory development and scientific computing with the opportunity to work closely with experimentalists and benefit from strong collaboration with an international partner with close interests.