Novel Magnetic Behavior in Thin Films and Ribbons

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An essential aspect of the search for novel magnetic materials is understanding the role of magnetism in determining other properties. Density functional calculations can play an important role by providing information about the properties of stable and unstable phases, including how they interact with other materials or are affected by dimensionality. Calculations are now routinely used to scan over a large numbers of possible candidate materials to find ones with specific properties. Alternatively, the “old fashion” approach of focusing on one particular material can also provide insights into the underlying physics with broader implications; this talk will discuss results using this latter approach for FeSe.

The normal state properties of superconducting FeSe monolayers present a quandry: experimentally there is no long-range magnetic order – making DFT calculations difficult – but the observed bands are reasonably well described by DFT calculations assuming the checkerboard antiferromagnetic ordering despite this configuration not being the calculated ordered ground state. We will discuss how treating the paramagnetic state as an incoherent superposition of spin-spiral states leads naturally to a magnetically disordered paramagnetic ground state, provides an explanation for the experimental ARPES data, and suggest that Néel fluctuations play a more important role in the electronic properties, including superconductivity, than previously appreciated. Similarly, the presence of edges (which can give rise to surface/edge electronic states) and impurities can modify the energetics of competing magnetic phases, with significant consequences on the overall properties, such as the formation of 1D superconducting edges in $FeTe_{1-x}Se_x$ ribbons.