# Theory-assisted search for novel itinerant magnets

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Our understanding of magnetism is based on two opposite perspectives. In the local moment picture, long-ranged magnetic order develops owing to exchange interactions between local moments carried by individual atoms. In the alternative itinerant view, an unpolarized conduction electron sea exhibits a correlation driven Stoner-type magnetic instability leading to a local imbalance of up- and down-spins. While the local moment magnetism was readily explained early on, the itinerant behaviour is still only poorly understood. The main limitation is a small number of known materials that are close to the itinerant limit. So far only three magnetic materials made of nonmagnetic constituents were discovered: two ferromagnets ($Sc_3In$, $ZrZn_2$) and one antiferromagnet (TiAu).

In this project, you will search for consecutive itinerant magnetic systems. You will start with performing first-principles electronic structure calculations aiming at choosing candidate compounds for experimental studies. Attempts to synthesize the selected materials will be carried using methods available in the Synthetic Solid State Physics lab at UCLan. Structural and compositional characterization of produced samples will be performed using diffractometers and electron microscopes available at the UCLan and will be followed by basic physical properties measurements in a dry cryostat at temperatures down to 4 K.

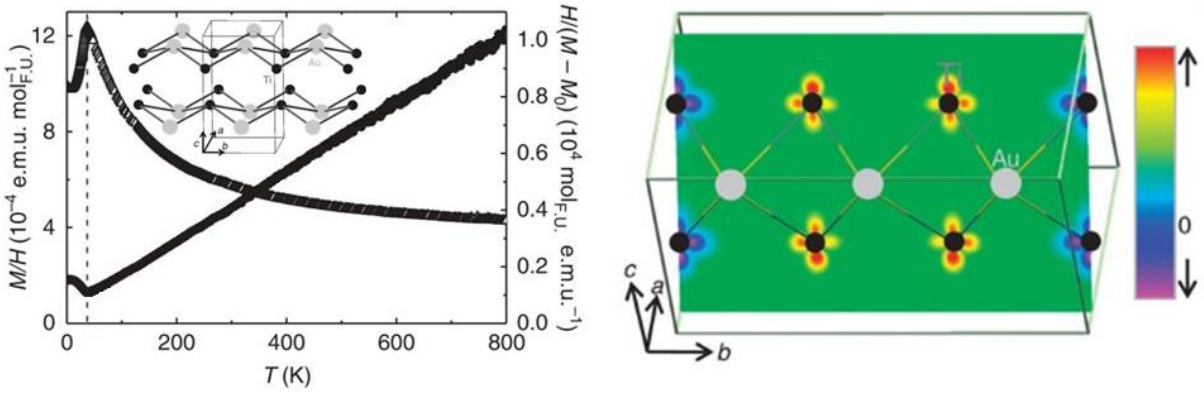


Figure 1: The left panel shows magnetic susceptibility as a function of temperature (left axis) and the inverse susceptibility (right axis) for TiAu measured in applied magnetic field of 0.1 T. The crystal structure of TiAu is displayed with the orthorhombic unit cell outlined in thin black lines. The right panel presents the electron spin density modulated along the *b* axis. The colour scale indicates degree of spin polarization (taken from [1]).

[1] E. Svanidze, J.K. Wang, T. Besara, L. Liu, Q. Huang, T. Siegrist, B. Frandsen, J.W. Lynn, A.H. Nevidomskyy, M.B. Gamża, M.C. Aronson, Y. Uemura and E. Morosan, Nature Communications **6**, 7701 (2015).