# A dynamical mean field theory study of self assembled diluted solids composed of strongly correlated d- and f- elements on a substrate

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We endeavour to investigate the properties of self assembled dilute super-lattices of d- and f-orbital elements on a metallic surface, within a fully self consistent DFT+DMFT (Dynamical Mean Field Theory) framework, that is able to fully capture the local strong correlations of magnetic rare earth and transition metal elements while also being able to capably converge the total electronic density.

We are motivated in this task by the experimental realization of a stable Ce super-lattice on Ag(111) [1]. Such a system is a promising candidate for the development of nanoscale magnetic memory devices, where the ad-atom states could possibly be controlled independently, allowing atomic scale information storage. Such devices are a subject of interest in academic and industrial sectors, with IBM successfully storing data using anti-ferromagnetic arrangements of Fe atoms [2]. This was done by individually placing atoms using an STM tip, but achieving success through self assembly mechanisms is obviously a desirable progression.

This is a difficult problem due to the multitude of possible phenomena at play. Experimental data suggests that the Kondo effect plays a role in the low electron density regime, and screening of the magnetic moment is indeed expected of the highly localised f-electron of Ce. There is the possibility of indirect exchange between the moments on adatoms giving rise to RKKY interactions, and a previous tight binding study has shown the importance of the ionic potential [3].

With all these possible effects present, it has been necessary to develop an advanced DMFT model using exact diagonalisation and cluster DMFT techniques to correctly take them all into account, and adequately treat the strongly localised d- or f-electron. These methods come with considerable computational costs, and so work has also been done to optimize the algorithms used.

While motivated by the Ce/Ag(111) lattice, our developing framework is universal and parameters can easily be changed to study numerous possible super-lattices of different transition and rare earth elements, on a variety of substrates. We hope that this can eventually be used as guiding tool for experimentalists, able to predict where in a complex phase space of temperature, adatom and substrate elements and competing interaction regimes, stable super-lattices might form and what regions of this space warrant further investigation.

[1] F. Silly et al, Phys. Rev. Lett., 92:016101, 2004

[2] Loth et al, Bistability in Atomic-Scale Antiferromagnets, Science 13 January 2012

[3] M. Ternes et al, Scanning-Tunneling Spectroscopy of Surface-State Electrons Scattered by a Slightly Disordered Two-Dimensional Dilute "Solid": Ce on Ag(111), 2004