

## Development of DFT methods to study atomic structure and pressure effects in f- electron materials

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Hello, my name is Julie Staunton.

I'm a professor in the theory group here at Warwick in the Physics department. I'm keen to recruit a HetSys PHD student to work on this project.

On the computational modelling of materials with the effect of f electrons are important. The project will involve some theory analysis as well as computational code development. The materials we will focus on contain rare earth or lanthanide elements, That's lanthanum through to lutecium. They're shown here on the periodic table.

Compounds involving them have many and varied applications, and it's particularly the case where strong magnets are required. The elements are interesting in that they all have similar chemistry owing to their common valence electronic structure, but different numbers of newly bound f electrons which determine magnetic properties amongst other things.

In this project we are going to use recent advances from alloy and magnetism theory for non rare earth materials to develop the widely used computational modelling methodology of density functional theory to describe lanthanide alloys with multi components and incorporate the f electron effects.

In this context cerium rich alloys are particularly fascinating. So cerium is over here. A cerium atom has just one f electron, so in most materials it behaves as if it is localised atomically in an atomically banned state, like the f electrons in all the other lanthanide elements.

However, in some chemical environments or under pressure, the f electron can propagate throughout the material, IE become band like, enjoying the valence electrons. This can trigger a remarkable change in the properties of the material.

In the latter stages of the project, there might be scope to build a machine learned interatomic potential for an appropriate serum alloy for further modelling.

Anyway, thanks for listening and your interest.