

4 PhD thesis fellowships in Condensed-Matter Physics (theory or experiments)

The theses will be financed by the joint French-German ANR-DFG grant “Fermi-Nest” (Fermi-surface topology and emergence of novel electronic states in strongly correlated electron systems).

Each PhD student will spent approximately 18 months in France and 18 months in Germany. These exchanges involve joint agreements between German and French universities and double PHD diplomas are expected. Two PhD projects will be jointly supervised by the two theoreticians who coordinate this FermiNEst project, G. Zwicknagl (g.zwicknagl@tu-bs.de), and S. Burdin (Sebastien.burdin@u-bordeaux.fr), with a central motivation: performing a realistic modelling of the materials that are investigated by the experimental partners of the project. Two PhD projects strengthen the experimental teams, in particular for performing quantum oscillation measurements, crystal growth and Raman spectroscopy. Detailed description of each thesis project and coordinates of PhD supervisors are provided hereafter:

Theory : Realistic modelling of unconventional orders in correlated electron materials

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The PhD project is dedicated to the realistic modelling of unconventional orders, that include homogeneous, modulated or chiral spin-liquids, exotic superconducting states like Fulde-Ferrell-Larkin-Ovchinnikov (FFLO), and anomalous fluctuations. In a first stage, the PhD student will be hosted in Bordeaux and he/she will study model Hamiltonians focusing on the specific properties and order parameters that may characterize unconventional orders. He/she will use mean-field methods which are appropriate for describing the highly correlated electronic states that involve f-orbitals. He/she will analyze the specificities of the Fermi Surface topologies that are expected to result from various kinds of unconventional orders. This phenomenological approach will be carried in close interaction with experimental teams. The idea is that a systematic analysis of the Fermi Surface topology in systems like URu₂Si₂, YbRh₂Si₂, or CeRu₂Si₂ under magnetic field, and CeCu₂Si₂ or CeRh₂Si₂ under pressure, should provide some strong constraints on the symmetries of the underlying mean-field like order parameters. In a second stage, after having identified possible mean-field like local or non-local order parameters for these compounds, the PhD student will perform appropriate band structure calculations. For these realistic quantitative calculations, he/she will be hosted in Braunschweig. In this project, the PhD student will learn band structure calculations under supervision of G. Zwicknagl, and mean-field approximations for correlated states under supervision of S. Burdin.

Theory: Electronic properties of correlated electrons in stoichiometric lanthanide compounds and substitutional alloys

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The central goal of this PhD project is to extend the Renormalized Band scheme to the calculation of the full 4f-electron spectral function at finite temperatures and to non-periodic substitutional alloys.

In a first stage, hosted in Braunschweig, the PhD student will learn electronic band structure calculation methods and their adaptations for taking into account correlation effects. An important part will be the efficient approximate solution of the quantum impurity problem including Crystal Electric Field effects as seen e.g. in Angle Resolved Photoemission Spectroscopy (ARPES). Trial compounds to begin with may be rare-earth “122” compounds, in particular CeNi₂Ge₂ for which the band structure has already been analyzed by G. Zwicknagl. Then, calculating the band structure of rare-earths “115” e.g. CeCoIn₅ by including correlation effects will provide new relevant results. In a second stage, during his/her stay in Bordeaux, the PhD student will study substitution effects, by combining Density Functional Theory (DFT) calculations and an appropriate dynamical mean-field method developed by S. Burdin. The substitutional series Ce_xLa_{1-x}Ni₂Ge₂ will be studied first, with a strong focus onto the non-Fermi liquid regime that was found experimentally in a large range of concentrations x. Cerium/rare-earth substitution effects in the 115 compounds mentioned above will then be studied.

Experiments: Investigation of strongly correlated electron systems by quantum-oscillation measurements

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The PhD project is dedicated to quantum-oscillation studies of strongly correlated electron systems in high magnetic fields. Such measurements are the tool-of-choice for the determination of the Fermi-surface topology in metals. In strongly correlated electron systems, high magnetic fields are usually required to observe quantum oscillations. In addition, high magnetic fields often induce electronic phase transitions. Among them are quantum phase transitions, i.e., continuous zero temperature phase transitions, around which new quantum phases are expected to emerge. Theoretically, such phase transitions are often accompanied by a Fermi-surface reconstruction. This is one of the key questions that will be addressed experimentally within this PhD project. The student will have a unique opportunity to use state-of-the-art high-field facilities of the European Magnetic Field Laboratory. This includes steady fields to 36 T and beyond available in Grenoble, France and Nijmegen, the Netherlands, as well as pulsed fields beyond to 70 T and higher in Dresden, Germany. All the measurements will be performed at low temperatures. This PhD project is part of a larger French-German collaboration, within which the student will be in contact with theoreticians, who will provide band-structure calculations to be compared with the experiment.

Experiments: Synthesis and crystal growth of Kondo lattice systems with strong Crystal Electric Field (CEF) effects

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This PhD project under the main supervision of C. Geibel is dedicated to the search for and the preparation, crystal growth and basic study of systems showing evidence for a strong involvement of the excited Crystal Electric Field (CEF) levels in low temperatures properties, especially in view of meta-orbital transitions. Since some of the compounds of interest for this topic are forming strongly peritectically (e.g. CeCoSi, CeCu₂Si₂), an important part of the project shall be to improve solid state recrystallization techniques. This technique shall be extended to further appropriate compounds of interest for the whole project, and is thus expected to extend its material basis. In the search part of the PhD project the work shall initially focus on a thorough study of CeCoSi. We shall then include further compounds we suspect to be of interest in the context of meta-orbital transition. In the crystal growth part, work shall initially concentrate on the recrystallization growth of CeCu₂Si₂, but further systems (e.g. CeCoSi, CeTiGe) shall follow soon. Study of the physical properties of the prepared samples and single crystals shall be an important part of this PhD project. Since Raman spectroscopy is likely an optimal technique to study CEF excitations under varying conditions, we plan to widely use this method to study the systems prepared within this PhD project. Therefore, we intend the PhD student to learn and participate into these Raman measurements. Therefore, the PhD student shall spend a total period of one year in Grenoble in the group of M.A. Measson.