Final Close-Out Report for DE-FG02-99ER45761

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For the FY Period
April 15th 1999 - February 14th 2020

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Abstract

This is a final close-out report for DOE contract DE-FG02-99ER45761 entitled "Correlation Effects and Magnetism in Actinides: Elements and Compounds" at Rutgers University in New Jersey. It funded condensed matter physics basic energy science research from 04/15/1999 through 02/14/2020. A list of postdocs that received support from this grant are presented below, along with an overview of the research accomplishments of the grant with highlights of research results from the last funding period and a list of original papers published thru the duration of the grant with impact factor metrics are presented.

Overview

The DOE Basic Energy Sciences grant "Correlation Effects and Magnetism in Actinides: Elements and Compounds" supported the research of professor Gabriel Kotliar at Rutgers, the State University of New Jersey. The objective of the project was to develop the basic theory needed to describe the solid state properties of actinide materials actinides (materials where the 5f shell is progressively filled), and to test the theory by comparing its outcome against existing experiments and by making new predictions. The concepts and techniques developed in this grant, are now used by many researchers . Forty publications resulted from this research and they received 4730 citations of May 6th, 2020.

The problem that initially drove our research can be exemplified by one archetypical elemental solid, Pu, the sixth member of the actinide series, which has been referred to as "an element at odds with itself". The solid state properties of this material, were not well described by the theoretical methods available when our research program was initiated.
For example, all the traditional electronic structure calculations, such as the standard implementations of density functional theory, underestimated the volume of the cubic phase (delta phase) of this material by about 30 %, when carried out in a non magnetic state. On the other hand, if the magnetic solutions are allowed, all forms of spin density functional theory predicted delta Pu to be magnetic with a magnetic moment of the order of 5 Bohr magnetons. No such static moment has been observed experimentally. Every other property of this phase was very mysterious, such as negative thermal expansion, very large specific heat and resistivities.

The initial project began in collaboration with E. Abrahams and J. R. Schrieffer, who were working on a model inspired by the classical work of Maria Gopper Mayer on the electronic structure of atoms, who had found that, in actinide materials, the Thomas Fermi potential had two minima, suggesting that multiple minima could exist once many body effects were taking into account in the solid. We proposed to develop that many body electronic structure method, DFT+DMFT (density functional theory plus dynamical mean field theory) to see if this method,

which combined quantum chemistry with band theory methods, could elucidate some of the mysteries of elemental plutonium and, more generally, of 5f elements and compounds.

The research funded by this grant advanced the basic energy science needed to understand by developing new concepts, new theoretical and computational methods, and by computing experimental consequences of the theory (theoretical spectroscopies) amenable to experimental tests. Besides the numerical computations we developed simple qualitative pictures of the actinides to intuitively understand their properties.

We summarize below in broad strokes the main accomplishments of this grant, and then in more detail the result of the last funding period. We divide our developments in three periods.

In the first period [1999 – 2006], the grant focused on energetics, and used very simplified impurity solvers in the DMFT equations. The goal was to obtain correct lattice constants assuming a paramagnetic state. We approached the actinides as strongly correlated materials. The theory not only accounted for the correct lattice constants of delta Pu in a non-magnetic framework, but also predicted the phonon spectra of delta Pu, which was later measured in inelastic neutron scattering experiments. Several anomalies, such as the degeneracy of optical and acoustic modes, were computed and measured. We established that the occupation number of f electrons was slightly bigger than 5 in agreement with x-ray absorption measurements. The relevance of concepts connected with the Mott transition placing delta Pu at the border between itinerant and localized behavior and connections with the ideas of the Invar model were explored.

The second period [2006 – 2012] focused on magnetism and spectroscopy. It introduced more advanced impurity solvers for the solution of the DMFTA equations. Magnetically ordered states of elemental actinides were explored and shown to be stable for Curium but not for Plutonium, which was now firmly established to be paramagnetic. The type of strong correlations involved in this material was refined to the notion of a mixed valent state. Tools to study aspects of magnetism, such as form factors induced by a magnetic field, were developed within DMFT, as well as tools to compute XAS branching ratios. New concepts such as quasiparticle multiplets and DMFT histograms were developed and provided an underpinning to the concepts of valence in the solid state. It was shown that multiplet splittings determine the width of the Hubbard bands in materials such as Americium. Successful comparisons with photoemission experiments were carried out in several actinide compounds and the presence of satellite features which we dubbed quasiparticle multiplets was shown to be a signature of mixed valence in photoemission.

The third period [2013 – 2020] broadens the scope of our studies to study multiple compounds and more complex phases of elemental plutonium. A new basic concepts was necessary to describe the results of our study: orbital, and site differentiation. There was a paradigm shift from Mott-induced correlations to Hund-induced correlations. We searched for approximate solvers that could be of use to approach more complex material science posed by actinides problem. Finally, several reviews that were written to clarify the new perspectives brought by our work on the actinide problem. The theory predicted signatures of mixed valence in the

neutron scattering spectra, in the form of a resonance below 100 meV. This was observed experimentally in neutron scattering experiments at ONRL.

Below we report in more detail on the work carried out in the last funding period of the grant September 2016 – September 2019 with a six-month no-cost extension to February 2020. In this period the following goals were accomplished.

1) Elucidated the nature of the correlations in the 5f series, particularly the role of Hund coupling in addition to the Hubbard U, as well as the roles of site and orbital differentiation in actinides.
2) Continued experimental collaborations to advance the goal of a theoretical spectroscopy of 5f materials. The scope of those collaborations broadened from elemental solids to actinide compounds.
3) Continue to explore simpler alternatives of the LDA+DMFT method, such as the rotational invariant slave boson method (RISB) and simplified cluster schemes for multiorbital systems.

Highlights of Research (October 2016 - February 2020)

The research accomplishments in this period, resulted in ten publications in refereed journals. We divide the resulting papers in four categories:

1. Theory of orbital differentiation in actinides,
2. Theory-experiment interactions
3. Exploring new methodologies
4. Dissemination in review articles

Theory of orbital differentiation in actinides

In [7], we advanced our investigation of compounds. The goal was validating codes against experiments while simultaneously gaining new physical insights into actinide-complex materials. We studied the normal state of the superconducting compound PuCoGa5 using the combination of density functional theory (DFT) and dynamical mean-field theory (DMFT), with the continuous time quantum Monte Carlo (CTQMC) and the vertex-corrected one-crossing approximation (OCA) as the impurity solvers. Our DFT+DMFT (CTQMC) calculations suggest a strong tendency of Pu-5f orbitals to differentiate at low temperatures. The renormalized 5f5/2 states exhibit a Fermi-liquid behavior whereas one electron in the 5f7/2 states was at the edge of a Mott localization. We found that orbital differentiation is present in this compound, affecting a removal of the 5f7/2 spectral weight from the Fermi level relative to its DFT value. We corroborated these conclusions with DFT+DMFT (OCA) calculations which demonstrate that 5f5/2 electrons have a much larger Kondo scale than the 5f7/2. This discovery of orbital differentiation was very unexpected and it should have enormous implications for spectroscopies which probe unoccupied states.

In [5], we investigated the electronic structure of the highly anisotropic β phase of metallic plutonium within the combination of density functional theory (DFT) and dynamical mean field theory (DMFT). Its crystal structure gives rise to site and orbital selective electronic correlations, with coherent Pu-5f5/2states and very incoherent Pu-5f7/2states. Hund's coupling is essential in determining the strength of correlations in Pu-5fstates. It is also responsible for the quasiparticle multiplets features in the Pu-5fspectral function.

Theory-experiment interactions.

Significant effort was placed in interactions with experiment, to test to what degree theory can serve as a theoretical spectroscopy. In [2], theory discovered a new extreme form of orbital differentiation whereby some orbitals undergo Kondo effect and form heavy quasiparticles, while others are magnetically ordered, due to the RKKY interaction. That RKKY behavior and Kondo behavior can coexist simultaneously in the same material was a surprising theoretical idea, which is strongly supported by tunneling experiments carried out in Pegor Aynajian's group.

In [1], we explored the physics of the 5f^2 system USb2 which has been of recent interest due to the discovery of rich proximate phase diagrams and unusual quantum coherence phenomena.

Here, linear-dichroic X-ray absorption and elastic neutron scattering are used to characterize electronic symmetries on uranium in USb2 and isostructural UBi2. Of these two materials, only USb2 is found to enable strong Hund's rule alignment of local magnetic degrees of freedom, and to undergo distinctive changes in local atomic multiplet symmetry across the magnetic phase transition.

Postdoctoral associate connected with our grant provided theoretical support for the Center for Actinide Science and Technology directed by Thomas E. Albrecht Schmitt. Calculations using the RISB method developed in the previous funding period [11] were carried out by current and former postdocs on a series of trivalent f-block tungstates, $MW_2O_7(OH)(H_2O)$ (M = La, Ce, Pr, Nd, and Pu) and $AmWO_4(OH)$. In [3] we demonstrated that the optical properties do not stem directly from the 5f electrons, as in both systems the valence band has mostly O-2p character and the conduction band has mostly W-5d character. Furthermore, the quasi-particle gap is essentially unaffected by the 5f degrees of freedom. Despite this, our analysis demonstrates that the f-electron covalency effects are quite important and substantially different energetically in $PuW_2O_7(OH)(H_2O)$ and $AmWO_4(OH)$, indicating that the optical gap alone cannot be used to infer conclusions concerning the f electron contribution to the chemical bond in these systems.

Exploring new methodologies

We presented [9] a formulation of quantum molecular dynamics that includes electron correlation effects via the Gutzwiller method. Our new scheme enabled the study of the dynamical behavior of atoms and molecules with strong electron interactions. The Gutzwiller approach goes beyond the conventional mean-field treatment of the intra-atomic electron repulsion and captures crucial correlation effects such as band narrowing and electron localization. We use Gutzwiller quantum molecular dynamics to investigate the Mott transition in the liquid phase of a single band metal and uncover intriguing structural and transport properties of the atoms. This is a toy model, and this calculation is simply a proof of principle. Still, to our knowledge, this is the first quantum molecular dynamic simulation which directly includes Mott Hubbard physics. It provides further support for the idea that temperature dependent force fields are necessary to capture the physics of this class of materials. ([16] formulated the same in a previous funding period of this grant).

In [4], we benchmarked ground-state calculations of the one- and two-dimensional Hubbard model utilizing the cluster extensions of the rotationally invariant slave-boson mean-field theory and the density matrix embedding theory. Furthermore, we propose a unified computational framework that allows us to implement both of these techniques on the same footing. This provides us with a different line of interpretation and paves the ways for developing systematically distinct generalizations of these complementary approaches which are needed when DMFT methods become prohibitively expensive. Ref. [10] proposed a cluster scheme for multiorbital systems of potential applicability to f compounds and tested in iron based systems.

Review Articles

Some of the research achievements of this grants were reviewed in two prestigious publications. [6] will be a standard reference on the properties of Plutonium for the years to come. With P. Soderlind (Livermore), we wrote the theoretical chapters reviewing the physics of actinides and strong correlation effects in the heavy actinides were highlighted.

[8] was written with Paul Kent for the prestigious Journal of Science and displays the synergies of this grant with existing DOE Centers for Materials Science.

The results on Plutonium supported by this grant were used to highlight many unique aspects of correlated materials which at this point cannot treated by any correlated method except for Dynamical Mean Field Theory.

Human Resources Development

Over a twenty year period our grant at different times provided support to postdoctoral associates. They continued to have careers in academia, industry and administration. We list their current employment below: Thomas Ayral (staff scientist Atos), Xi Dai (currently professor in Hong Kong Technical University) , Xiaoyu Deng (employed in the finantial industry), Chang-Jong Kang (postdoctoral associate Rutgers), Nicola Lanatà (professor Aharus University), Chris Marianetti (professor at Columbia University), Maria Pezzoli (administrator ICTP) Jihoon Shim (professor at Postech), Sergej Y. Savrasov (currently professor at UC Davis), Zhiping Yin (professor Normal University Beijing).

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Tsung-Han Lee, Thomas Ayral, Yong-Xin Yao, Nicola Lanata, and Gabriel Kotliar
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212 citations as of May 6th, 2020

Total number of citations: 4730 as of May 6th, 2020

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