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Russian Contract Procurement Document

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April 1, 2010

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This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Statement of Work

Sponsoring Program	Lawrence Livermore National Laboratory ASC Program (Advanced Simulation and Computing)		
CIS Institute or Company Name:	Federal State Unitary Enterprise "Russian Federal Nuclear Center – Zababkhin All-Russia Research Institute of Technical Physics (FSUE "RFNC-VNIITF")	Complete Mailing Address: 13 Vasilyeva, Snezhinsk, Chelyabinsk Region, 456770 Russia	
Contract Type (check one)	Participating MPC&A Institute <input checked="" type="checkbox"/> or For Profit Company <input type="checkbox"/>		
Director of the Institute	Georgy Rykovanov, Director, RFNC-VNIITF		
SOW Title:	Study of Relativistic Discrete Variational (RDV) Methods		
WBS #, Project Title and Annex 1 Number Required for all MPC&A Contracts	Same as MTA # B512530	Total Estimated Cost of SOW	\$100,000
Lead Author/Point of Contact at Institute:	Alexey Mirmelstein	Phone #	+7-(35146)
		Fax #	+7-(35146)
		E-mail:	mirmelstein@mail.ru
POC Address if different than Institute/ Company	Russian Federal Nuclear Center-Institute of Technical Physics 13 Vasilyeva, Snezhinsk, Chelyabinsk Region, 456770 Russia		
LLNL Requestor/PI Contact:	James G. Tobin	Phone #	925-422-7247
		Fax #	925-423-7040
		E-mail:	Tobin1@LLNL.Gov

This contract supports the enhancement of physical protection or nuclear material control and accounting systems at institutes or enterprises of the newly independent states under the material protection control and accounting (MPC&A) program. The contract is entered into pursuant to the MPC&A Program, a gratuitous technical assistance program, in accordance with the bilateral Agreements between the Russian Federation and the United States of America concerning the Safe and Secure Transportation, Storage and Destruction of Weapons and the Prevention of Weapons Proliferation of June 1992, as extended and amended by Protocol signed of June 1999, Agreement between the Government of the Russian Federation regarding Cooperation in the Area of Nuclear Materials Physical Protection, Control and Accounting of October 1999 and the Russian Federation law of May 1999 on the taxation exemption of gratuitous technical assistance with Russian Federation under registration #DOE001000.

Description of Work

1.0 Objective (What and Why)

Provide a brief statement that identifies the building or activity (training, sustainability, etc.) on which work is to be performed. The objective should also state what the purpose of the work is.

The work in terms of this agreement will promote investigations in physics of f-electron materials in the Institute, implementation of new experimental methods, involvement of new partners, and participation of the Institute members in International conferences. Contract will run for one year, beginning on the agreed start date.

When all tasks have been completed, three individuals from VNIITF and lower-tier Institutes shall visit LLNL. VNIITF covers all expenses connected with this visit (travel including local, accommodation, meals) for its employees, and power-tier Institutes for their employees. During this visit the results obtained in terms of the contract should be discussed, as well as perspectives for future collaboration.

"RFNC-VNIITF" PI: Alexey Mirmelstein

The problem of ground state of plutonium metal is one of the central problems in modern solid state physics. In recent years this element has been the focus of both theoretical and experimental investigations. In spite of the considerable progress in the field of both theory (calculations of the electron structure) and experiments, many questions regarding the physics of plutonium remain unanswered, including those concerning the number of electrons in its f shell, clear understanding of its magnetic properties, and the driving forces of structural phase transition in plutonium.

Elegant XAS and EELS experiments performed by LLNS group have shown the f-count $N_f \sim 5.2$ in both alpha- and delta- phases of plutonium metal [see, e.g., JG Tobin et al., J. Phys.: Condens. Matter 20 (2008) 125204]. Also, very similar N_f value follows from DMFT electronic spectrum calculations by Shim et al. [JH Shim et al., Nature 446 (2007) 513]. At the same time an approach to describe magnetic susceptibility and specific heat of plutonium based on the concept of multiple intermediate valence (MIV) indicates N_f to be less than 5 in both Pu phases [A. Mirmelstein et al., JETP Letters 90 (2009) 485]. Obviously, both approaches meet severe restrictions. The atomic multi-electron model by G. van der Laan et al. used to analyze XAS and EELS spectra does not account for the reality of a solid state sample. On the other hand, the empirical MIV model can also be too simplified since it is based on the theoretical equations developed for the "ordinary" intermediate-valence systems fluctuating between two electronic configurations, and requires further development and verification. A direct way to improve our understanding of Pu properties would be to extend van der Laan's atomic model by for the case of a solid state sample. However, it is extremely difficult to incorporate into the atomic model non-integer filling of the f-states which follows from almost any electronic structure calculation for the materials of our interest.

In order to gain new insight into the electronic properties of Pu in the present work another approach can be suggested which is based on the cluster consideration of the system under study. Relativistic Discrete Variational (RDV) method will allow us to follow modification of atomic states as a function of the number of ions in the cluster. By the other words, it is possible to understand systematically how the atomic states transform when going from an isolated atom to a solid. Potentially, as a second step, effect of ionization may also be considered. In principle, from these cluster calculations it can be possible to derive independent estimate of the f-count and, perhaps, to obtain new basis for further development of absorption spectra calculations.

Experimental study of such important actinides' properties as bulk modulus, compressibility and phase stability as a function of external pressure are of great interest. To be able to perform these investigations, RFNC-VNIITF is developing now an experimental facility for X-ray diffraction measurements in a diamond anvil cell.

Thus the following work is to be performed in terms of the contract between Lawrence Livermore National Laboratory, Russian Federal Nuclear Center – Russian Research Institute of Technical Physics (RFNC-VNIITF), Snezhinsk, and the following Lower Tier Subcontractors: Institute of Solid State Chemistry, Russian Academy of Sciences, Ural branch, Ekaterinburg, Institute of Nuclear Research, Russian Academy of Sciences, Moscow:

I. Theoretical part. The RDV cluster calculations of the electronic configuration of fcc plutonium metal.

I.1. The RDV investigation of the fully relativistic electronic and chemical bonding structures as well as electronic configuration of plutonium atoms in Pu_2 dimer- **the 1st quarter of the project execution.**

These calculations will show the variation of Pu atomic states due to the formation of plutonium dimer. Influence of dimer size (Pu-Pu distance) on the electronic configuration will be investigated. Similar calculations will also be performed for Np and Am, plutonium neighbors in the Periodic table. This may be important for qualitative understanding of unique features of Pu electronic structure.

I.2. The RDV investigation of the chemical bonding structure and atomic orbital (AO) populations for the central Pu atom in Pu_{19} cluster which geometry and boundary conditions correspond to the fcc δ -Pu lattice – **the 2nd quarter of the project execution.**

Obviously, these calculations constitute the second step in studying the transformations of atomic states when going from an isolated atom to a solid, since the coordination number of Pu is increased from 1 to 12 in this case. Therefore, these calculations take into account the interaction of Pu atom with its nearest neighbors

I.3. The RDV investigation of the electronic structure of large Pu₇₉ and Pu₂₀₁ clusters with crystal-lattice boundary conditions – **the 4th quarter of the project execution.**

These calculations allow to follow transformations of atomic states when going from the first coordination sphere of the central plutonium atom to second and third neighbors. Thus, this step provides more realistic picture of Pu electronic states in a solid.

The RDV method is based on the solution of the Dirac-Slater equation for 4-component wave functions transforming according to the irreducible representations of the double point groups representing the symmetry of molecules or clusters. For the calculation of symmetry coefficients the original code will be used which realizes the projection-operators technique. The extended bases of four-component numerical atomic orbitals (AO) obtained as the solution of the Dirac-Slater equation for the isolated neutral atoms, also includes Pu7p_{1/2} and 7p_{3/2} functions, in addition to the occupied AOs. The degree of Pu5f, 6d, 7s, 7p states delocalization could be evaluated by the values of overlap populations of various pairs of atomic orbitals n_{ij} of the neighboring Pu sites. The overlap populations can also give the bond orders of these states. The values of n_{ij} for 5f-5f, 5f-6d, 6d-6d, 5f-7s and 6d-7s AOs can show the detailed structure of chemical bonding in the system under study.

II. Experimental part. Development of experimental facilities for basic research of actinides: installation of X-ray powder diffractometer with Imaging Plate detector and diamond anvil cell, calibration and test experiments.

II.1. Installation and testing of X-ray powder diffractometer equipped with diamond anvil cell - **the 1st quarter of the project execution.**

Since this is a new experimental technique for the RFNC-VNIITF group, this step includes necessary training in operation with Almax-Boehler type of diamond anvil cell (DAC) up to ~ 30 GPa pressure as well as test measurements to calibrate pressure (using, e.g., NaCl as a pressure standard).

II.2. Study of the pressure effects on the crystal structure and phase transitions of intermediate-valence compound CeNi - **the 2nd quarter of the project execution.**

CeNi is a well known intermediate-valence system. The RFNC-VNIITF group performed a series of experiments to study effects of chemical and external pressure on the properties of CeNi [A. Mirmelstein et al., *J. Alloys. Comp.* **444&445** 281-284 (2007), A. Mirmelstein et al., *J. Nucl. Mater.* **385** 57-59 (2009)]. Using neutron diffraction measurements it was shown that only two CeNi phases exist within pressure-temperature domain (T < 300 K, P < 2 GPa), namely, the orthorhombic ambient-pressure and the tetragonal high-pressure ones. Thus, the planned experiments constitute a continuation of the study of pressure effects in CeNi to determine the low-pressure phase crystal lattice parameters as a function of pressure. The task includes also further attempts to determine the space group of the high-pressure phase of CeNi which remains to be unknown.

The most interesting pressure range for these experiments does not exceed ~ 5 GPa. However, efforts are to be undertaken to extend the measurements up to ~ 30 GPa for training reasons.

II.3. Study of the pressure effects on the crystal structure of the chemically compressed CeNi-based compositions Ce_{1-x}Lu_xNi (x < 0.2) – **the 3rd quarter of the project execution.**

The goal of this study is the same as in item II.2, but for chemically compressed composition. Existence of a pressure-induced phase transition is questionable in this system.

II.4. Test experiments to study pressure effects on the structure of U-based materials - **the 4th quarter of the project execution.**

The aim of previous measurements includes both scientific and methodical components since they provide necessary experience in operation with DAC. Experiments with U-based materials are required to test experimental ability of the instrument to work with highly-absorbing samples. This is the main goal of item II.4.

The reports on the work performed are to be submitted each half a year of the contract execution. The results are to be presented at the international conferences (e.g. Plutonium Future – The Science 2010 and/or other related meetings) and published in pre-reviewed scientific journals.

List of the main participants from Russian side.

1. Dr. Alexey Mirmelstein, principal investigator, RFNC-VNIITF, contact person.
2. Yuri Zuev, Head of Department, RFNC-VNIITF
3. Oleg Kerbel, technical staff, RFNC-VNIITF
4. Vladimir Matvienko, technical staff, RFNC-VNIITF
5. Alexander Shestakov, Head of X-ray diffraction group, RFNC-VNIITF
6. Igor Artamonov, technical staff, X-ray diffraction group, RFNC-VNIITF
7. Konstantin Toporishchev, technical staff, X-ray diffraction group, RFNC-VNIITF
8. Alexander Sedov, technical staff, X-ray diffraction group, RFNC-VNIITF
9. Dr. Evgeny Clementyev, Institute Nuclear Research, Russian Academy of Sciences, Moscow
10. Prof. Dr. Alexander L. Ivanovskii, Head of Lab, Inst. of Solid State Chemistry, Russian Academy of Sciences, Ekaterinburg
11. Dr. Igor Shein, senior scientist, Institute of Solid State Chemistry, Russian Academy of Sciences, Ekaterinburg
12. Dr. Michael Ryzhkov, senior scientist, Institute of Solid State Chemistry, Russian Academy of Sciences, Ekaterinburg.

LaborPricing for each task shall be supported in the following format:

Task 1 (first and second quarter)

Labor Category	Man-Month Rate in US\$	No. of Man-Months	Extended Price in US\$
VNIITF Staff			
Principal Investigator	1,200	1	1,200
Lead Research Associate	900	1	900
Lead Engineer	800	4	3,200
Research Associate			
Engineer	400	11	4,400
Technician			
Economist	600	0.833	500
Laborers (Worker)			
Interpreter/Translator	600	0.5	300
Administrative (Clerical Worker)			
Total			10,500
ISSC Staff			
Principal Investigator	1,200	6	7,200
Lead Research Associate	900	6	5,400
Lead Engineer			
Research Associate	800	0.8	640
Engineer			
Technician			
Economist	600	0.6	360
Laborers (Worker)			
Interpreter/Translator			
Administrative (Clerical Worker)			
Total			13,600
INR Staff			
Principal Investigator			
Lead Research Associate	900	3	2,700
Lead Engineer			
Research Associate	800	1.25	1,000
Engineer			
Technician			
Economist	600	0.5	300
Laborers (Worker)			
Interpreter/Translator			
Administrative (Clerical Worker)			
Total			4,000

Task 2 (third and fourth quarter)

Labor Category	Man-Month Rate in US\$	No. of Man-Months	Extended Price in US\$
VNIITF Staff			
Principal Investigator	1,200	1	1,200
Lead Research Associate	900	1	900
Lead Engineer	800	4	3,200
Research Associate			
Engineer	400	11	4,400
Technician			
Economist	600	0.833	500
Laborers (Worker)			
Interpreter/Translator	600	0.5	300
Administrative (Clerical Worker)			
Total			10,500
ISSC Staff			
Principal Investigator	1,200	6	7,200
Lead Research Associate	900	6	5,400
Lead Engineer			
Research Associate	800	0.8	640
Engineer			
Technician			
Economist	600	0.6	360
Laborers (Worker)			
Interpreter/Translator			
Administrative (Clerical Worker)			
Total			13,600
INR Staff			
Principal Investigator			
Lead Research Associate	900	3	2,700
Lead Engineer			
Research Associate	800	1.25	1,000
Engineer			
Technician			
Economist	600	0.5	300
Laborers (Worker)			
Interpreter/Translator			
Administrative (Clerical Worker)			
Total			4,000

Total

Labor Category	Man-Month Rate in US\$	No. of Man-Months	Extended Price in US\$
Principal Investigator	1,200	14	16,800
Lead Research Associate	900	20	18,000
Lead Engineer	800	8	6,400
Research Associate	800	4.1	3,280
Engineer	400	22	8,800
Technician	-	-	-
Economist	600	3.866	2,320
Laborers (Worker)	-	-	-
Interpreter/Translator	600	1	600
Administrative (Clerical Worker)	-	-	-
Total			56,200

2.3 Deliverables: *This table should specify briefly (one line) the expected deliverable(s), the number of months after award of the agreement that the deliverable is expected, and the amount that will be paid when the deliverable is accepted. If a task has subtasks, then a deliverable and the amount to the payment for that deliverable must be specified for each subtask.*

The Institute shall prepare all reports in both English and Russian. Reports shall be submitted electronically by e-mail. If reports can only be submitted in paper form then the Institute shall identify this requirement in advance and mail the documents to the Lawrence Livermore National Laboratory. A list of the required deliverables is defined in the chart below.

Item	Description	Delivery Due
Task 1 Deliverable	Report on details of first and second quarter results	Six months after receipt of award
Task 2 Deliverable	Report on details of third and fourth quarter results	Twelve months after receipt of award

3.0 Seller Acquired Property

All PI's should get the following information, in this form, signed and sealed by the institute to speed the requisition process. Specifications for non-Russian equipment should be obtained in one of two forms: 1) specification sheets, or 2) specifications on a signed and sealed letter from the institute. If the specifications are considered national security information (e.g., some Eleron sensors) this should be noted and procurement will evaluate the best course of action.

Please make the equipment description a generic term: a ViewSonic Monitor should be referred to as simply a monitor. If possible utilize the exact words in the commodities list of the International Cooperative License.

There is no need to fill the itemized list out if you have the signed quote from the institute attached. Just note that the equipment list is attached and enter the total estimated cost in the space below.

Description	Manufacturer	Make & Model Number	Vendor	Country of Origin	Qty	Unit Price in US\$	Total Price in US\$
Boehler µDriller		EMC& LDV compliant for Europe	easyLab Technologies Ltd.	UK	1	22,500	31,400 including vat, custom, and shipment
Total							31,400

The Boehler µDriller is a fully-automated electro-discharge-machine system that enables the drilling of precision holes in a gasket material required to perform high-pressure experiments in diamond anvil cells.

Total Estimated Cost of SAP: \$31,400

Is a quote for SAP from the institute attached (Yes/No)? Y

Travel

Pricing for travel that your Institute requires to perform the work described in the SOW shall be supported in the following format:

Departure and Arrival Locations	No. of trips	No. of Travelers	Misc. in US\$	Transport cost per traveler in US\$	No. of Travel days	Daily lodging cost per traveler in US\$	Daily meal cost per traveler in US\$	Extended Price in US\$
Ekaterinburg-Keystone(Colorado, USA)-Ekaterinburg Pu Futures – The Science 2010	1	1		2,000	7	120	60	4,000 including conference fee
Ekaterinburg-Livermore-Ekaterinburg	1	3		2,000	5	100	60	8,400
Total								12,400

Total Estimated Cost of Travel: \$12,400

5.0 Misc. Services (interpreters, equipment rental, etc.)**Total Estimated Cost of Misc. Services: \$0****6.0 University Furnished Equipment: none**

Are requisitions for UFE being submitted at the same time: No

Deliverable Structure

The final report should be in English and Russian. The report and draft shall be transmitted both electronically and on paper. The electronic version of the report can be either transmitted by electronic mail or on a disk in Microsoft Word format. Draft versions of the report should be provided one month before the official due date. The US will provide comments within 10 business days. The Russian Facility shall identify all proprietary information with appropriate visual markings. Information not identified as proprietary shall be considered non-proprietary.

Delivery

The Seller agrees to deliver as shown above after authorization to proceed. Such authorization shall only be in the form of an Order issued and signed by LLNL's Procurement Department. Delivery is in months after authorization to proceed.

EXPORT CONTROL DATA SHEET

1. Procurement Information

- a. P.O./Requisition Information:
 - a. Requisition #:
 - b. Contract/P.O. #:
 - c. Modification #:
 - d. Procurement Representative for contract:
- b. Is the request for labor or funds transfer only?
 - a. Total dollar amount:

2. General Information

- a. Name of PI/ Technical Consultant responsible for contract: James G. Tobin
- c. PI/Technical Consultant Telephone Extension: X27247
- d. LLNL Sponsoring Program: ASC Program (advanced simulation and computations)
- e. Project Names and WBS # (Required for MPC&A): Same as MTA # B512530
- f. Task Title (SOW Title): Study of Relativistic Discrete Variational (RDV) Methods

3. Export Destination (Required for MPC&A)

- a. Facility/Ultimate Site Consignee (name, address w/area, bldg., room): Russian Federal Nuclear Center-Institute of Technical Physics , 13 Vasilyeva, Snezhinsk, Chelyabinsk Region, 456770 Russia
- b. Lead Author/Point of contact for Consignee (individual, address w/area, bldg, room, phone): Alexey Mirmelstein, Russian Federal Nuclear Center-Institute of Technical Physics , 13 Vasilyeva, Snezhinsk, Chelyabinsk Region, 456770 Russia, **Phone #**+7-(35146)
- c. Is this facility involved in activities described in paragraph 4a below, whether or not those activities are related to this export?

Yes No (FOR MPC&A THE ANSWER IS ALWAYS YES)

4. End Use

- a. Specific End Use/User Statement (provide a brief description of the end use/users; note if individuals/facilities involved are Russian military or nuclear weapons related):
N/A – No equipment is being shipped, only funds.
- b. Does the intended end use of this equipment fall within (1) through (4) below?
N/A – No equipment is being shipped, only funds.
 - (1) Nuclear explosive activities, including research on or development, design, manufacture, construction, testing or maintenance of any nuclear explosive device, or components or subsystems of such a device.
 - (2) Activities including research on or development, design, manufacture, construction, operation, or maintenance of any nuclear reactor, critical facility, facility for the fabrication of nuclear fuel, facility for the conversion of nuclear material from one chemical form to another, or separate storage installation, where there is no obligation to accept International Atomic Energy Agency (IAEA) safeguards at the relevant facility or installation, when it contains any source or special fissionable material (regardless of whether or not it contains such material at the time of export).
 - (3) Safeguarded and unsafeguarded nuclear fuel cycle activities, including research on or development, design, manufacture, construction, operation or maintenance of any of the following facilities, or components for such facilities:
 - I. Facilities for chemically processing irradiated source or special nuclear materials;
 - II. Facilities for production of heavy water;
 - III. Facilities of the separation of isotopes of source or special nuclear materials; or
 - IV. Facilities for fabrication of nuclear reactor fuel containing plutonium.
 - (4) Research on or development, design, manufacture, construction, testing or maintenance of missiles, other delivery methods, chemical/biological weapons or agents, or nuclear propulsion.

PI/Technical Consultant Signature James G. Tobin

Date: 22/March/2010

SUPPLIER INFORMATION FORM
(only for contracts ≥\$100k)

I. COMPETITIVE SOLICITATION-not applicable

II. NON-COMPETITIVE SOLICITATION

- A. Identity of proposed sole/single-source supplier and socio-economic status:
VNIITF, Russia
- B. Basis for Reason: (see Requisition Instructions)
Russian defense lab

The above information is accurate and complete to the best of my knowledge and belief:

The undersigned acknowledges that in participating in this procurement action he or she does not reasonably expect the award of this procurement action to impact his or her financial interests or the financial interest of his or her immediate family.

Requester's Signature  Date 22March/2010

Requester's Name and Employee Number: James G. Tobin, 896032

