



IAEA

Atoms For Peace

الوكالة الدولية للطاقة الذرية

国际原子能机构

International Atomic Energy Agency

Agence internationale de l'énergie atomique

Международное агентство по атомной энергии

Organismo Internacional de Energia Atómica

MUSHARAF Ali
Bhabha Atomic Research Centre
Chemical Engineering Division
Trombay
400085 Mumbai
India

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E-mail: Official.Mail@iaea.org • Internet: <http://www.iaea.org>

In reply please refer to: RC-24055-R0

Dear Mr Musharaf,

2020-06-26

In accordance with previous correspondence on the subject, I take pleasure in sending you IAEA Agreement No. 24055/R0 concerning Research Project: "Atomistic Modeling of Permeation of Hydrogen Isotopes through Fe, W, Cu, and Cr" which is to be carried out at your institute free of charge to the IAEA.

If the terms and conditions mentioned in the agreement are acceptable to your institute, I should be grateful if you would have it signed by the person legally entitled to sign for your institute and return it to the Research Contracts Administration Section.

We are pleased to have the opportunity to cooperate with you and look forward to learning of the results of your work.

Yours sincerely,

Mr Sasha DAMJANAC
Head, Research Contracts Administration Section
Dept. of Nuclear Sciences & Applications



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Atoms For Peace and Development

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IAEA Research Agreement No: 24055/R0

Research Agreement

This Research Agreement is entered into between the International Atomic Energy Agency (hereinafter referred to as the "IAEA"), an intergovernmental organization established by its Statute, whose address is Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria; and the Bhabha Atomic Research Centre (hereinafter referred to as the "Institute") whose address is:

Bhabha Atomic Research Centre
Trombay
Mumbai 400 085
India .

Hereinafter, the IAEA and the Institute will also be referred to individually as a "Party" and collectively as the "Parties".

WHEREAS, the IAEA, in the implementation of its statutory function of encouraging and assisting research on, and development of practical application of atomic energy for peaceful uses, desires to extend the opportunity of participating in Coordinated Research Projects to research institutes in Member States, in order to assist in broadening the contact between the personnel of such institutes having similar interests and to offer these institutes scientific consultation and support;

WHEREAS, the Institute desires to participate in the Coordinated Research Project referred to in Article 1 ("Scope of the Research Project") of this Agreement;

NOW, THEREFORE, the Parties hereby agree as follows:

Article 1

Scope of the Research Project

1. The Institute undertakes to perform the Research Project entitled 'Atomistic Modeling of Permeation of Hydrogen Isotopes through Fe, W, Cu, and Cr' (hereinafter referred to as the "Research Project") which forms part of the IAEA Coordinated Research Project 'F43025' entitled 'Hydrogen Permeation in Fusion-Relevant Materials' (hereinafter referred to as the "CRP").
2. The Chief Scientific Investigator shall be Mr Musharaf, Ali.
3. The programme of the work to be performed under this Research Project shall be:

The proposal from Bhabha Atomic Research Centre (BARC) comprises of state-of-the-art quantum mechanical computations applied with electron density functional theories (DFT) to study the parameters effecting hydrogen fuel permeation in nuclear fusion wall materials. Parameters studied

are: hydrogen isotope adsorption, recombination, absorption, diffusion and effective permeation in the most important fusion materials relevant to this CRP namely W, Fe, Cu and Cr. The obtained parameters will comprise a well-defined database, which will be further applied in larger scale simulations using classical Molecular Dynamics calculations. Using this methodology by combining quantum mechanical results with classical simulations, provides understanding of the underlying physical phenomena to the larger scale events and even predictions of hydrogen permeation.

4. The programme of work may be further detailed by exchange of letters between the Parties.

Article 2

Duration of the Research Project

The Research Project shall commence on the date of the last signature by the duly authorized representatives of the Parties and shall continue until 01 September 2025. It may be extended for further periods through mutual written agreement of the Parties.

Article 3

Exchange of Information

The IAEA shall include the Institute in any reciprocal exchanges of information arranged by the IAEA among the institutes participating in the CRP, and shall invite it to participate in any meetings convened by the IAEA for institutes participating in that project.

Article 4

Reporting

The Institute agrees to submit a Report, in English language, to the IAEA of the work relating to the CRP for presentation at each Research Coordination Meeting held under the CRP and to assist other participants in the CRP when necessary.

Article 5

Publications

1. The Institute agrees that the IAEA may, while giving due recognition to the author(s), publish in the original language and other languages and make freely available, the reports to be submitted by the Institute to the IAEA further to Article 4 ("Reporting") of this Agreement. In order that the results arising out of this Research Project may be made available for the development and practical application of atomic energy for peaceful purposes throughout the world, the Parties agree to cooperate in the prompt and extensive publication of such reports.

2. In publishing any results of this Research Project, the Institute and its staff shall indicate that the Research Project was part of the CRP carried out under the sponsorship of the IAEA.

Article 6

Assignment

The Institute shall not assign, transfer, pledge or make other disposition of this Agreement or any part thereof or of any of the Institute's rights, claims, liabilities or obligations under this Agreement except with the prior written authorization of the IAEA.

Article 7

Indemnification

The Institute shall indemnify, hold and save harmless and defend, at its own expense, the IAEA, its officials, agents and employees, from and against all suits, claims, demands and liability of any nature

or kind, including their costs and expenses, arising out of: (i) acts or omissions of the Institute or its employees in the performance of this Agreement, including claims and liability in the nature of workmen's compensation claims; and (ii) claims arising out of the unauthorized use of patented inventions or devices, copyrighted material or other intellectual property provided by the Institute under this Agreement.

Article 8

Use of name, emblem or official seal of the IAEA

Except as provided in paragraph 2 of Article 5 ("Publications") of this Agreement, the Institute shall not advertise or otherwise make public the fact of its relationship with the IAEA. Furthermore, the Institute shall, in no other manner whatsoever use the name, emblem or official seal of the IAEA or any abbreviation of the name of the IAEA in connection with its business or otherwise.

Article 9

Officials Not to Benefit

The Institute warrants that it has not and shall not offer to any representative, official, employee, or other agent of the IAEA any direct or indirect benefit arising from or related to the performance of this Agreement or of any other agreement with the IAEA or the payments thereof or for any other purpose intended to gain an advantage for the Institute. The Institute agrees that breach of this provision may lead, at the IAEA's sole discretion, to the annulment of this Agreement irrespective of any work performed. The annulment shall exclude any right of the Institute to claim any payment, even for work already performed. The annulment will be without prejudice to any further remedies that the IAEA may be entitled to under this Agreement or at law, with particular reference to refund of payments already made, claims for damages and losses occurred, bribery, and fraud. The provisions under this Article shall also apply with respect to any subcontractor for the part of work related to such subcontractor.

Article 10

Audit

Any payment made by the IAEA shall be subject to audit by auditors, whether internal or external, of the IAEA or by other authorized and qualified agents of the IAEA at any time during the term of this Agreement and for a period of five (5) years following the expiration or prior termination of this Agreement. The IAEA shall be entitled to a refund from the Institute for any amounts shown by such audits to have been paid by the IAEA other than in accordance with the terms and conditions of this Agreement.

The IAEA may conduct audits or investigations relating to any aspect of this Agreement or any payments made in connection with this Agreement, the obligations performed under this Agreement, and the operations of the Institute generally relating to performance of this Agreement at any time during the term of this Agreement and for a period of five (5) years following the expiration or prior termination of this Agreement.

The Institute shall provide its full and timely cooperation with any such inspections, post-payment audits or investigations. Such cooperation shall include, but shall not be limited to, the Institute's obligation to make available its personnel and any relevant documentation for such purposes at reasonable times and on reasonable conditions and to grant to the IAEA access to the Institute's premises at reasonable times and on reasonable conditions in connection with such access to the Institute's personnel and relevant documentation. The Institute shall require its agents, including, but not limited to, the Institute's attorneys, accountants or other advisers, to reasonably cooperate with any inspections, audits or investigations carried out by the IAEA hereunder.

Article 11
Observance of Law

The Institute shall comply with all laws, ordinances, rules, and regulations bearing upon the performance of its obligations under this Agreement.

Article 12
Status of Institute

The Institute shall have and maintain the legal status of an independent contractor. The personnel of the Institute shall not be entitled to act as an agent of the IAEA.

Article 13
Privileges and Immunities

Nothing in this Agreement shall be construed as a waiver of the privileges and immunities accorded to the IAEA by its Member States.

Article 14
Force Majeure

1. Force majeure as used in this Article shall mean any unforeseeable and irresistible act of nature, any act of war (whether declared or not), invasion, revolution, insurrection, terrorism, industrial and/or civil disturbances, formal orders of local courts and authorities or any other act of a similar nature or force, provided that such acts arise from causes beyond the control of a Party and without the fault or negligence of that Party.
2. In the event of and as soon as possible after the occurrence of any cause constituting force majeure, the Institute shall give notice and full particulars in writing to the IAEA of such occurrence or change if the Institute is thereby rendered unable, wholly or in part, to perform its obligations and meet its responsibilities under this Agreement. The Institute shall also notify the IAEA of any other changes in conditions or the occurrence of any event which interferes or threatens to interfere with its performance of the Agreement. On receipt of the notice required under this Article, the IAEA shall take such action as, in its sole discretion, it considers to be appropriate or necessary in the circumstances, including the granting to the Institute of a reasonable extension of time in which to perform its obligations under the Agreement.
3. If the Institute is rendered permanently unable, wholly or in part, by reason of force majeure to perform its obligations and meet its responsibilities under this Agreement, the IAEA shall have the right to suspend or terminate this Agreement on the same terms and conditions as are provided for in Article 19 ("Termination"), except that the period of notice shall be seven (7) days instead of thirty (30) days.

Article 15
Survival

The obligations set forth in Articles 5 ("Publications"), 13 ("Privileges and Immunities), and 16 ("Settlement of Disputes") of this Agreement shall not cease upon termination of this Agreement.

Article 16
Settlement of Disputes

All disputes arising out of or relating to interpretation or implementation of this Agreement, which cannot be amicable settled by the Parties, shall be referred by either Party to arbitration for settlement in accordance with the UNCITRAL Arbitration Rules as in force at the date the dispute is referred to

arbitration. The number of arbitrators shall be one. The place of arbitration shall be Vienna, Austria. The language of arbitration shall be English. The decisions of the arbitrator shall be final and binding on the Parties.

Article 17
Entry into Force and Duration

This Agreement shall enter into force on the date of the last signature by the duly authorized representatives of the Parties and remain in force until the Parties have discharged their obligations hereunder, unless terminated earlier pursuant to the terms of this Agreement.

Article 18
Amendment

No modification of, or changes to, this Agreement, or waiver, either expressed or implied, of any of its provisions shall be valid unless made in writing and approved by the duly authorized representatives of the Parties.

Article 19
Termination

Either Party may for valid cause terminate this Agreement, in whole or in part, upon thirty (30) days' prior written notice to the other Party. Where notice of termination is given, the Institute shall, as appropriate, take immediate steps to bring the work and services under this Agreement to a close in a prompt and orderly manner.

For the IAEA:

Mr Sasha DAMJANAC
Head, Research Contracts Administration Section
Dept. of Nuclear Sciences & Applications

Date: 26 June 2020

For the Institute:
(Head of the Institute)

के जयकुमार/K Jayakumar
अध्यक्ष, योजना एवं समन्वय प्रभाग
Head, Planning & Coordination Division
ज्ञान प्रबंधन बर्ग, मा प अ केंद्र/KMG, BARC
भारत सरकार/Government of India
ट्रॉम्बे, मुंबई/Trombay, Mumbai -400 085.

Date: 17/7/2020