

भाभा परमाणु अनुसंधान केंद्र का आधिकारिक द्विमासिक प्रकाशन
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हाइड्रोजन
उत्पादन
प्रौद्योगिकियाँ

Hydrogen
Generation
Technologies



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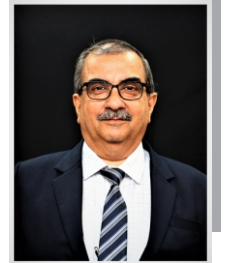
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नाभिकीय विज्ञान का राष्ट्रीय हाइड्रोजन मिशन के साथ एकीकरण

जीवाश्म ईंधन और विकारबनीकरण क्षेत्रों जैसे शोधन, उर्वरकों एवं अन्य पर निर्भरता को कम करने के लिए हाइड्रोजन इस लीग में, एक महत्वपूर्ण स्वच्छ ऊर्जा वाहक के रूप में उभर रहा है। इस उल्लेखनीय कायान्तरण (परिवर्तन) के आलोक में, भाभा परमाणु अनुसंधान केंद्र (भा.प.अ. केंद्र) ने हाइड्रोजन उत्पादन, नाभिकीय एकीकरण और भंडारण को शामिल करते हुए अनुसंधान एवं प्रौद्योगिकीय विकास कार्य का एक व्यापक दायरा शुरू किया है। न्यूज़लेटर का यह अंक इस क्षेत्र में जारी विकास कार्यों को प्रदर्शित करने हेतु समर्पित है।



हमारा प्रमुखता से ध्यान स्वदेशी जल-अपघटन प्रौद्योगिकियों के विकास पर है। भा.प.अ. केंद्र ने प्रयोगशाला-स्तरीय प्रणालियों से लेकर औद्योगिक-स्तरीय इकाइयों तक क्षारीय जल वैद्युत-अपघटक (एडब्ल्यूई) उन्नत किए हैं, जिसमें हाइड्रोजन उत्पादन हेतु $10 \text{ Nm}^3/\text{h}$ प्रौद्योगिकी पहले से ही उद्योग भागीदारों को हस्तांतरित की गई है। प्रगत केशिका और संकर प्राकृतिक-परिसंचरण वैद्युत-अपघटक के साथ-साथ स्वदेशी प्रोटॉन एक्सचेंज मेम्ब्रेन (पीईएम) प्रौद्योगिकी पर कार्य जारी है, जो इस क्षमता को अधिक सुदृढ़ बना रहा है। इसकी एक अन्य आशाजनक विधि उच्च तापमान वाला वाष्प विद्युत अपघटन है, जिसमें भा.प.अ. केंद्र नाभिकीय ठोस-ऑक्साइड विद्युत अपघटन सेलों का विकास कर रहा है और 800°C पर स्थिर प्रचालन का प्रदर्शन कर रहा है।

ऊष्मा-रासायनिक चक्र उच्च तापमान ऊष्मा का उपयोग करके बड़े पैमाने पर हाइड्रोजन उत्पादन के लिए एक और मार्ग प्रशस्त करता है। आयोडीन-सल्फर (आई-एस) चक्र को इसके बंसेन, सल्फ्यूरिक-अम्ल अपघटन और हाइड्रोजन-आयोडाइड अपघटन खंडों में व्यवस्थित प्रगति के साथ विकसित किया जा रहा है, जिसका उद्देश्य एक एकीकृत बंद-लूप प्रक्रिया प्राप्त करना है। कल्पाकृम में, कॉपर-क्लोरीन (Cu-Cl) चक्र निरंतर बेंच-स्केल प्रचालन से 150 NL/h प्रायोगिक सुविधा तक आगे बढ़ा है। भा.प.अ. केंद्र, विशाखापट्टणम में प्रस्तावित 5 MWth उच्च-तापमान गैस-शीतित उच्च तापमान रिएक्टर के साथ इसका नियोजित एकीकरण नाभिकीय-सहायता प्राप्त हाइड्रोजन उत्पादन का प्रदर्शन करने की दिशा में एक महत्वपूर्ण कदम है।

लेखों में, हाइड्रोजन मान श्रृंखला अर्थात भंडारण के एक महत्वपूर्ण हिस्से को भी दर्शाया गया है। 2-डी नैनो-पदार्थों पर शोध यह रहस्योद्घाटित करता है कि किस प्रकार डोपिंग और तनाव प्रतिवर्ती हाइड्रोजन भंडारण को बढ़ा सकते हैं, जबकि ठोस-अवस्था पदार्थ धातु हाइड्राइड, उच्च-सतह-क्षेत्र पदार्थ और रासायनिक हाइड्राइड पर सुरक्षित, उच्च-घनत्व भंडारण विकल्पों के रूप में कार्य करते हैं।

इन गतिविधियों का यह संकलित रूप, राष्ट्रीय हाइड्रोजन मिशन में भा.प.अ. केंद्र के योगदान को दर्शाता है, जिसमें मूलभूत पदार्थ अनुसंधान और विद्युत रासायनिक प्रौद्योगिकियों से लेकर ऊष्मागतिकीय प्रक्रमों, नाभिकीय-ताप एकीकरण, अभियांत्रिकी प्रदर्शन और प्रौद्योगिकी हस्तांतरण तक शामिल हैं। यह प.ऊ.वि. अमृत काल विज्ञान 2047 के साथ संरेखित है, जो भारत के दीर्घकालिक ऊर्जा संक्रमण और प्रौद्योगिकीय आत्मनिर्भरता के महत्वपूर्ण घटकों के रूप में स्वच्छ हाइड्रोजन, प्रगत रिएक्टरों और स्वदेशी प्रौद्योगिकी विकास को रेखांकित करता है। यह कार्यक्रम प्रयोगशाला अनुसंधान से प्रदर्शन तक और अंत में, नाभिकीय-समर्थित हाइड्रोजन प्रौद्योगिकियों के बड़े पैमाने पर परिनियोजन की स्पष्ट प्रगति को दर्शाता है।

विवेक भसीन

श्री विवेक भसीन

निदेशक

भाभा परमाणु अनुसंधान केंद्र (भा.प.अ. केंद्र)

Integrating Nuclear with National Hydrogen Mission

Hydrogen is emerging as an important clean energy carrier for reducing dependence on fossil fuels and decarbonising sectors such as refining, fertilisers, and others in this league. In light of this remarkable transformation, Bhabha Atomic Research Centre (BARC) has undertaken a broad spectrum of research and technology development work encompassing hydrogen production, nuclear integration and storage. This issue of Newsletter is dedicated to showcasing the ongoing developmental work in this domain.



A major focus is the development of indigenous water-splitting technologies. BARC has advanced alkaline water electrolyzers (AWEs) from laboratory-scale systems to industrial-scale units, with technology for 10 Nm³/h hydrogen production already transferred to industry partners. Work on advanced capillary and hybrid natural-circulation electrolyzers, as well as indigenous Proton Exchange Membrane (PEM) technology is underway, further strengthening this capability. High-temperature steam electrolysis is another promising route, with BARC developing tubular solid-oxide electrolysis cells and demonstrating stable operation at 800°C.

Thermochemical cycles provide another pathway for large-scale hydrogen production using high temperature heat. The Iodine-Sulfur (I-S) cycle is being developed through systematic advances in its Bunsen, sulfuric-acid decomposition and hydrogen-iodide decomposition sections, with the objective of achieving an integrated closed-loop process. The Copper-Chlorine (Cu-Cl) cycle has progressed further, from sustained bench-scale operation to a 150 NL/h pilot facility at Kalpakkam. Its planned integration with the proposed 5 MWth high-temperature gas-cooled high temperature reactor at BARC, Visakhapatnam represents an important step towards demonstrating nuclear-assisted hydrogen production.

The articles also address a critical part of the hydrogen value chain i.e., storage. Research on 2-D nanomaterials explores how doping and strain can enhance reversible hydrogen storage, while work on solid-state materials probes metal hydrides, high-surface-area materials and chemical hydrides as safer, high-density storage options.

Taken together, these activities reflect BARC's contribution to National Hydrogen Mission cutting across fundamental materials research and electrochemical technologies to thermochemical processes, nuclear-heat integration, engineering demonstration and technology transfer. This aligns with the DAE Amrit Kaal Vision 2047, which identifies clean hydrogen, advanced reactors and indigenous technology development as important constituents of India's long-term energy transition and technological self-reliance (Aatmanirbharta). The programme demonstrates a clear progression from laboratory research to demonstration and, finally, large-scale deployment of nuclear-assisted hydrogen technologies.

A handwritten signature in blue ink, appearing to read 'Vivek Bhasin'.

Vivek Bhasin
Director

Bhabha Atomic Research Centre (BARC)

सतत हाइड्रोजन उत्पादन एवं भंडारण

वर्तमान प्रगति और भावी लक्ष्य

सह-संपादक
का संदेश

भा भा परमाणु अनुसंधान (भा.प.अ.) केंद्र न्यूज़लेटर में “हाइड्रोजन उत्पादन प्रौद्योगिकी” पर इस विशेषांक को प्रकाशित करते हुए हमें अत्यंत हर्ष की अनुभूति हो रही है। कार्बन उत्सर्जन को न्यूनतम करते हुए वैश्विक ऊर्जा मांग को पूरा करने में हरित ऊर्जा प्रौद्योगिकियां महत्वपूर्ण हैं। यह ‘नाभिकीय ऊर्जा मिशन’ के अंतर्गत निर्धारित भारत के महत्वाकांक्षी नेट ज़िरो संकल्प के साथ भी सुमेलित है। इस चुनौती से पार पाने में हाइड्रोजन एक आशाजनक ऊर्जा वाहक है। हालांकि, हाइड्रोजन का उत्पादन, कुशल हाइड्रोजन भंडारण विधियां, और हाइड्रोजन-आधारित अर्थव्यवस्था को विकसित करने के लिए ऊर्जा रूपांतरण उपकरणों में अंतिम उपयोग के लिए शिक्षाविदों और उद्योग के सभी हितधारकों के समन्वित कार्यों द्वारा समर्थित एक दीर्घकालिक दृष्टिकोण की आवश्यकता है। भाभा परमाणु अनुसंधान केंद्र (भा.प.अ. केंद्र) हाइड्रोजन उत्पादन, शुद्धिकरण, भंडारण और उपयोग हेतु प्रौद्योगिकियों के विकास पर अनवरत एवं ठोस प्रयास कर रहा है।

इस विशेषांक में, संयंत्र स्तर पर हाइड्रोजन उत्पादन, प्रयोगशाला पैमाने पर हाइड्रोजन भंडारण से लेकर हाइड्रोजन के कुशल भंडारण के लिए प्रथम मूल पदार्थ अभिकल्पन तक विषयों की विस्तृत श्रृंखला को समेकित करते हुए छः लेख प्रस्तुत किए गए हैं। हम, अत्यंत अल्पावधि में सभी लेखकों द्वारा इस विषय पर लेखों के माध्यम से योगदान करने हेतु आभार प्रकट करते हैं। इस न्यूज़लेटर का आरंभ निदेशक, भा.प.अ. केंद्र के प्राक्कथन से किया गया है। इस अंक में, जल अपघटन के माध्यम से स्वच्छ हाइड्रोजन के उत्पादन के लिए कॉपर-क्लोरीन (Cu-Cl) ऊष्मा-रासायनिक चक्र और ऊष्मा-रासायनिक आयोडीन-सल्फर (I-S) प्रक्रिया पर चर्चा की गई है। इसके बाद, कम तापमान वाले जल विद्युत अपघटन और उच्च तापमान वाले वाष्प विद्युत अपघटन का उपयोग करके हाइड्रोजन उत्पादन पर लेख प्रस्तुत किया गया है। इसके अलावा, प्रयोगों और पहले सिद्धांतिक गणनाओं का उपयोग करके प्रतिवर्ती हाइड्रोजन भंडारण हेतु विभिन्न प्रतिभागी पदार्थों पर चर्चा की गई है। कुल मिलाकर, ये सभी लेख हाइड्रोजन उत्पादन एवं भंडारण के लिए प्रौद्योगिकी विकास के क्षेत्र में अनेक व्यावहारिक ज्ञान प्रदान करते हैं। भा.प.अ. केंद्र न्यूज़लेटर का यह विशेष अंक भविष्य के लक्ष्यों के साथ-साथ टिकाऊ हाइड्रोजन उत्पादन और भंडारण में वर्तमान प्रगति पर प्रकाश डालता है।

हम इस अवसर पर श्री मनोज सिंह, अध्यक्ष, एसआईआरडी को और एसआईआरडी की संपादकीय टीम, विशेष रूप से, श्री माधव एन. को इस विशेष अंक के लिए सभी लेखों की विषय-वस्तु की रचना, अभिकल्पन और प्रमाणीकरण की तैयारी में उनकी कड़ी मेहनत और सत्यनिष्ठा के साथ किए गए प्रयासों के लिए आभार प्रकट करते हैं। हम, श्री कल्याण भांजा, सह निदेशक, रासायनिक इंजिनियरी वर्ग से प्राप्त सतत सहयोग और प्रोत्साहन के लिए उनके प्रति विशेष आभार व्यक्त करते हैं।


डॉ. सुलेखा मुखोपाध्याय
अध्यक्ष, रासायनिक इंजीनियरी प्रभाग


डॉ. शेख मुशरफ अली
रासायनिक इंजीनियरी प्रभाग

Sustainable Hydrogen Generation and Storage

Current Progress & Future Goals

It gives us immense pleasure to bring out this special issue on “Hydrogen Generation Technologies” in BARC Newsletter. Green energy technologies are vital for satisfying global energy demand while significantly lowering carbon emissions. This also aligns with India’s ambitious Net Zero directives set under ‘Nuclear Energy Mission’. Hydrogen is a promising energy carrier to address this challenge. However, production of hydrogen, efficient hydrogen storage methods, and ultimate usages in energy conversion devices to develop hydrogen-based economy calls for a long-term vision supported by coordinated actions from all stakeholders across academia and industry. Bhabha Atomic Research Centre (BARC) has been making persistent and concerted efforts for the development of technologies for hydrogen generation, purification, storage and utilization.

ASSOCIATE
EDITORS’
message

In this special issue, there are six articles covering wide range of topics from plant scale hydrogen generation, laboratory scale hydrogen storage to first principles materials design for efficient storage of hydrogen. We thank all authors for contributing articles for this issue on short notice. The newsletter starts with a foreword by Director, BARC. In this issue, Copper-Chlorine (Cu-Cl) thermochemical cycle and thermochemical Iodine-Sulphur (I-S) process for production of clean hydrogen through water splitting have been discussed. Next, hydrogen generation using low temperature water electrolysis and high temperature steam electrolysis has been presented. Further, different candidate materials for reversible hydrogen storage using experiments and first principles calculations are discussed. Overall, all these articles provide a great deal of practical knowledge in the field of technology development for hydrogen generation and storage. This special issue of the BARC Newsletter highlights current progress in sustainable hydrogen production and storage, along with future goals.

We take this opportunity to thank Shri. Manoj Singh, Head, SIRD and the Editorial Team of SIRD, in particular, Shri. Madhav N., for his hard work and sincere efforts in carrying out content curation, design and preparation of proofs of all the articles for this special issue. We sincerely thank Shri Kalyan Bhanja, Associate Director, Chemical Engineering Group for his constant support and encouragement.



Dr. Sulekha Mukhopadhyay
Head, Chemical Engineering Division



Dr. Sk. Musharaf Ali
Chemical Engineering Division

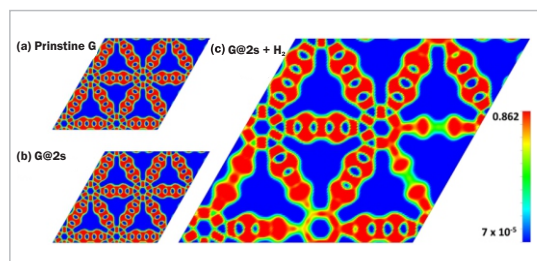
इस अंक में INSIDE...



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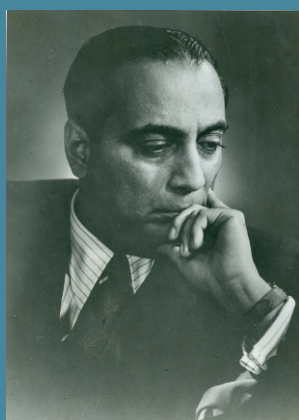
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आयोडीन-सल्फर ऊष्मा-रासायनिक प्रक्रिया का प्रौद्योगिकी विकास

Technology Development of Iodine-Sulfur Thermochemical Process

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सारांश

हाइड्रोजन एक आशाजनक स्वच्छ ऊर्जा वाहक के रूप में उभरा है जो पर्यावरणीय प्रभाव को कम करते हुए बढ़ती ऊर्जा मांगों को पूरा करने में सक्षम है। विभिन्न उत्पादन विधियों में, स्वच्छ ऊर्जा स्रोतों द्वारा संचालित ताप रासायनिक जल विभाजन को बड़े पैमाने पर हाइड्रोजन उत्पादन के लिए सबसे दीर्घकालिक दृष्टिकोणों में से एक माना जाता है। इस प्रक्रिया में, पुनःचक्रण योग्य मध्यवर्ती यौगिकों से जुड़ी रासायनिक अभिक्रियाओं के एक क्रम के माध्यम से पानी को हाइड्रोजन और ऑक्सीजन में अपघटित किया जाता है। जाँच किए गए कई तापरासायनिक चक्रों में, आयोडीन-सल्फर (आई-एस) चक्र ने अपनी उच्च दक्षता और उच्च तापमान ऊष्मा स्रोतों के साथ संगतता के कारण विशेष रूप से ध्यान आकर्षित किया है। आई-एस चक्र में तीन प्रमुख अभिक्रिया चरण शामिल हैं : बंसेन अभिक्रिया, सल्फ्यूरिक एसिड अपघटन और हाइड्रोजन आयोडाइड (एचआई) अपघटन। यह लेख इनमें से प्रत्येक चरण में प्रौद्योगिकीय प्रगति की समीक्षा करता है और एक पूरी तरह से एकीकृत, बंद-लूप आई-एस ताप-रासायनिक चक्र विकसित करने की दिशा में प्रगति पर प्रकाश डालता है। ये विकास बड़े पैमाने पर हाइड्रोजन उत्पादन के लिए एक स्थायी मार्ग के रूप में आई-एस प्रक्रिया की क्षमता को प्रदर्शित करते हैं।

ABSTRACT

There is an urgent need for an alternative energy carrier that can meet growing energy demands without posing a threat to the environment. Among the various clean energy options, hydrogen has emerged as one of the most promising and environmentally benign energy carrier. The most sustainable and attractive route for hydrogen production is the splitting of water using clean energy sources. Thermochemical water-splitting processes offer significant potential for large-scale hydrogen production. In these processes, water is decomposed into hydrogen and oxygen through a series of chemical reactions involving intermediate compounds that are continuously recycled within the cycle. Among the numerous thermochemical cycles investigated worldwide, the iodine-sulfur (I-S) thermochemical cycle is one of the most extensively researched due to its high efficiency and suitability for integration with high-temperature heat sources. The I-S process consists of three major reaction steps: the Bunsen reaction, sulfuric acid decomposition, and hydrogen iodide (HI) decomposition. This article discusses the technological developments achieved in each of these reaction sections and highlights the progress made toward the realization of a fully integrated closed-loop I-S thermochemical cycle for sustainable hydrogen production.

KEYWORDS: Iodine-Sulphur Process, Thermochemical, Hydrogen Energy



एचआई अपघटन अध्ययन हेतु व्यवस्था का चित्र।

HI decomposition setup

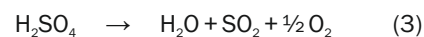
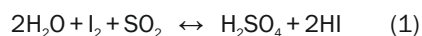
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Introduction

Fossil fuels are limited in supply and their use leads to greenhouse gas emissions. Hence there is a need to replace/limit the usage of fossil fuels with a clean fuel. Further the energy produced at the clean fuel source needs to be transported to the various end users. Apart from electricity, Hydrogen is seen as a clean energy carrier, if produced from water using non carbon based primary energy source [1]. There are many ways to produce hydrogen by splitting water, thermochemical methods are one such process. The thermochemical cycles are processes where water is decomposed into hydrogen and oxygen via chemical reactions using intermediate elements which are recycled. The sum of all the reactions is equivalent to the dissociation of the water molecule into hydrogen and oxygen. Thermochemical processes produce hydrogen by splitting water at far less temperatures in comparison to direct thermolysis of water. A number of thermochemical processes are studied to generate hydrogen from water, of this Iodine–Sulfur (I-S) process has been widely studied because of its high efficiency, scalability, all fluid process etc [1]. I-S process broadly consists of three steps (as shown in reaction 1, 2, and 3).

Thermochemical process consisting of three chemical reaction steps [2] which are shown below.



Reaction (1), called Bunsen reaction, produces two acids (hydriodic and sulfuric acid) via reaction with water, iodine and sulfur dioxide exothermically. Afterwards, produced HI_x and H_2SO_4 phases are separated and sent to the respective sections for production of H_2 and O_2 by reactions (2) and (3), respectively. I-S process involves highly corrosive chemicals [3], hence it becomes necessary to have corrosion resistance materials. As an important step toward the demonstration of the I-S process, Bhabha Atomic Research Centre (BARC) Mumbai, initiated extensive research and development activities on the process. Initially, a closed-loop I-S system was established using glass and quartz equipment operating at atmospheric pressure and prototypical temperature conditions. Since the process involves highly corrosive chemicals and severe operating environments, extensive corrosion studies were carried out successfully under representative process conditions.

Subsequently, individual reaction sections of the I-S process were studied using engineering materials to evaluate their long-term feasibility and material compatibility. Building upon these developments, a demonstration facility employing engineering materials has been established to realize and validate the closed-loop operation of the I-S thermochemical process for sustainable hydrogen production.

I-S Process in Glass/Quartz Setup

The initial development of a laboratory-scale closed-loop I-S thermochemical system to demonstrate continuous hydrogen production through water splitting is focused. The

overall process flow sheet was designed for a hydrogen production basis of 150 Nlph.

The closed-loop experimental setup was fabricated using glass, quartz based equipment and consisted of reactors, separators, purifiers, heat exchangers, and associated auxiliary components.

The development programme was carried out in a phased manner. Initially, individual equipment units were tested independently to evaluate their performance and operational stability. Subsequently, section-wise integrated experiments were conducted to study the interaction between interconnected equipment and to establish stable continuous operation of the process.

Based on the experience gained from equipment-level and section-wise experimentation, the fully integrated closed-loop glass system was operated successfully in continuous mode for 20 hours, achieving a hydrogen production rate of 30 Nlph. With this successful demonstration, India became the fifth country in the world—after the United States, Japan, South Korea, and China—to demonstrate continuous closed-loop operation of the I-S thermochemical cycle for hydrogen production. Fig.1 gives the integrated facility of I-S Process in glass/quartz setup. Fig.2 shows the temperature profile of various unit operations and processes during stable closed loop operation. Hydrogen is sampled periodically and analyzed using gas chromatograph and flow rate was analyzed using water displacement method periodically.

Material Testing Studies

Material identification issues are crucial for successful deployment of I-S process on large scale [3]. materials research areas relate to development of construction materials, and catalysts. Efforts are on to find solutions, which render the I-S process efficient and economical.

I-S Process involves highly corrosive and hazardous media. Identification of compatible material of construction would be a breakthrough in realization of technology. In order to identify compatible material of construction, corrosion test study has been done with special metals, ceramic, PTFE and



Fig.1: Closed loop glass/quartz I-S facility.



हाइड्रोजन उत्पादन प्रौद्योगिकियाँ HYDROGEN GENERATION TECHNOLOGIES

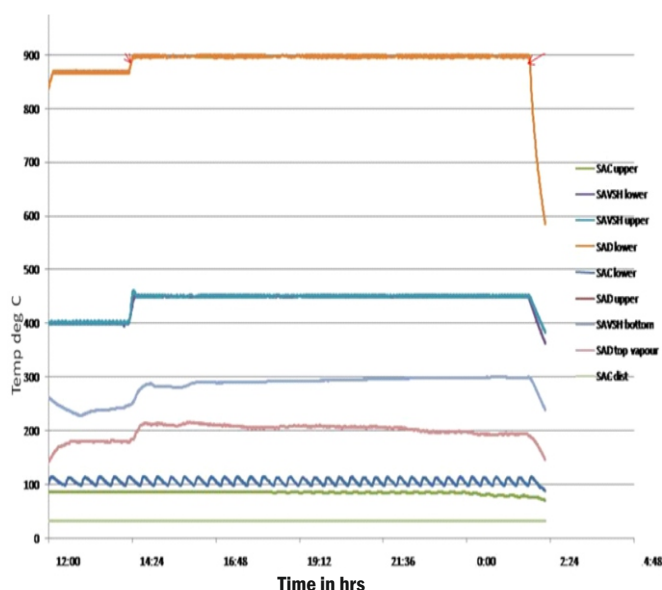


Fig.2: Temperature profiles during period of closed loop operation.

noble metals in actual chemical reaction environment in flowing streams for the development of I-S thermochemical process in metallic system.

Test coupons studied in the process are Incoloy 800H, Incoloy 800, Tantalum, Hastelloy-C276, Alloy 33, Molybdenum, Titanium, Niobium, Niobium-1% Zirconium, PTFE, Silicon Carbide, Platinum, Silver and Gold.

Bunsen Section

Metallic Bunsen system

Bunsen reaction constitutes one of the three main reaction steps of I-S [4].

Bunsen reaction is a multiphase, reversible and exothermic in nature as given in Fig.3 [5]. Reactor selection and design procedure should reckon this and exothermicity of the reaction in addition to the product quality and side reactions [4, 5].

Materials have been identified for individual sections of I-S Process after corrosion studies.

An experimental facility to study Bunsen reaction and phase separation is designed and installed. Elaborate

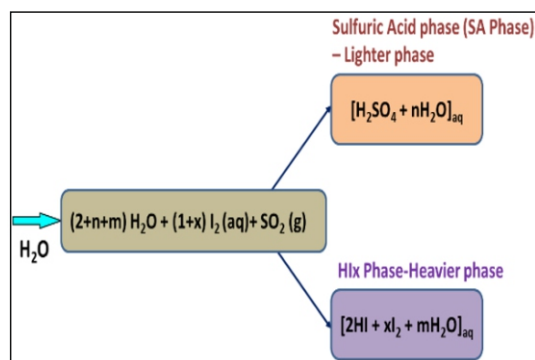


Fig.3: Bunsen reaction scheme with excess I_2 and H_2O .

Table 1: Typical summary of compatible material of construction in various equipments.

Equipment & temperature	Test Coupons							
	Incoloy 800H	Ta	Alloy C276	Ti	SiC	Pt	Ag	Au
SO_3 Decomposer & 900 °C	✓				✓	✓		✓
H_2SO_4 Decomposer & 500 °C	✓				✓	✓	✓	-
HI_x solution & 127-180 °C		✓			✓	-	-	-
HI decomposer & 500 °C		✓	✓	✓	✓	✓		✓
50 wt % H_2SO_4 & 122 °C	✓	✓	✓		✓	-	-	-
70 wt % H_2SO_4 & 167 °C	✓	✓	✓		✓	-	-	-
90 wt % H_2SO_4 & 260 °C		✓	✓		✓	-	-	-
HI vaporizer & 127 °C	✓	✓	✓	✓	✓	-	-	-

experimentation are carried out in the facility. The schematic of the setup is shown in Fig.4. The feed and reaction system are shown in Fig.5 & 6 respectively.

Operating conditions like temperature, composition etc. have to be optimally selected to achieve high purity of product phases, conversion [5].

Sulfuric Acid Decomposition Section

Thermal decomposition of sulfuric acid is, where high temperature heat input is required for endothermic reaction [6,7]. Decomposition involves three steps; Equation (4) represents sulphuric acid vaporisation or phase change step, takes place near 337 °C at atmospheric pressure condition.

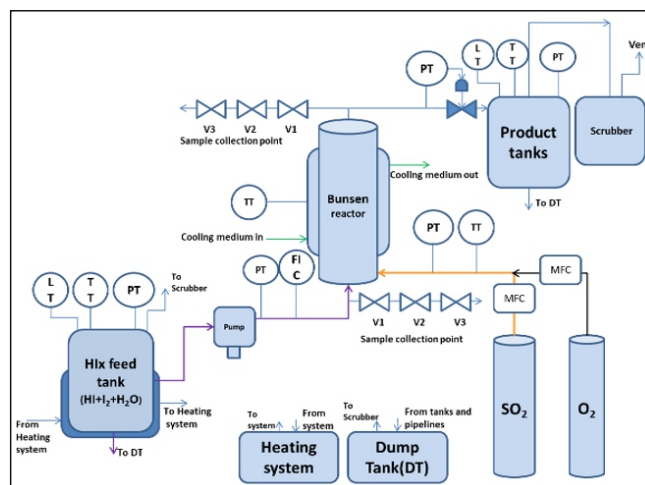


Fig.4: Schematic of Metallic Bunsen setup.

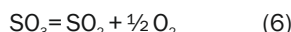
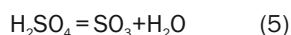


Fig.5: Feed system of Metallic Bunsen setup.



Fig.6: Bunsen reactor in Metallic Bunsen setup.

Eq (5) and (6) represent acid decomposition, at temperature up to 550 °C and sulfur trioxide decomposition, at 900 °C, respectively. Sulfur trioxide decomposition is the heterogeneous catalytic reaction step [7]. The schematic is shown in Fig.7



Chromium doped iron oxide catalyst, is found to be promising, active and stable mixed oxide catalyst for trioxide decomposition, a better alternate for Pt catalyst [6].

Activation energy and frequency factor of this catalyst are obtained during intrinsic reaction kinetic study with powder catalyst. Catalyst is found to be stable and hence considered for further studies [7].

HI Decomposition Section

HI decomposition is one of the important reaction step in I-S Process [2]. It is an endothermic catalytic reaction. Problems of HI section are azeotrope formation by HI_x mixture, lack of appropriate thermodynamic data and difficulty in decomposing HI. To break azeotrope H_3PO_4 was used by GA, USA. JAEA, Japan is focused on using EED (Electro-electro dialysis) combined with a H_2 permselective membrane reactor.

The HI_x solution, which is produced in the Bunsen process reactor, is nearly quasi-azeotropic. Application of the conventional distillation to separating HI from the solution is viable solution but energy intensive. Alternative distillation methods including the extractive distillation using phosphoric acid and the reactive distillation in pressurized condition have been investigated in literature [3]. In addition, application of membrane technologies has also been considered such as the pervaporation and the electro-membrane process called electro-electrodialysis (EED).

HI decomposition studies are carried out using conventional packed bed reactor. The setup is shown in Fig. 8.



Metallic Closed Loop I-S Process

BARC has been involved in technical demonstration of IS process. To achieve this target, a bench scale facility is set up in BARC, Mumbai.

The objective of the project is demonstration of a metallic closed loop I-S process system involving three sections at prototypical process conditions for hydrogen production at 150 Nlph at atmospheric pressure by using electrical heat and compatible materials of construction for various equipments. The schematic of the process is shown in Fig.9 and the facility in Fig.10.

Various issues cropped up which have been overcome during demonstration. The facility is commissioned and successfully demonstrated H_2 production at 150 Nlph capacity.

After successfully demonstrating I-S process in engineering materials, the process is scaled up to 3 m^3/h (3000 Nlph) hydrogen production capacity. This setup is coming up at HWB(M) facility and being worked out in collaboration with HWB. Modified I-S process is envisaged to decrease the highest temperature requirement of the I-S process from 850 °C to ~500 °C by eliminating sulphuric acid decomposition step. The SO_2 required in the Bunsen reaction can be provided from industries where it is generated or by combustion of sulphur itself.

It is proposed to utilize the high temperature heat from high temperature gas cooled reactor (HTGCR) which is being developed for demonstrating production of clean hydrogen using modified I-S process. Modified versions of the process wherein highest temperature step of the process can be avoided are being worked out with private vendors through Atal Incubation Center, Mumbai.

Summary

The realization of the hydrogen as an energy carrier for future energy relies on a practical method of producing hydrogen in large scale with no emission of greenhouse gases. In order to realize an industrial scale process, materials play a vital role. I-S process involves highly corrosive atmosphere.



हाइड्रोजन उत्पादन प्रौद्योगिकियाँ HYDROGEN GENERATION TECHNOLOGIES

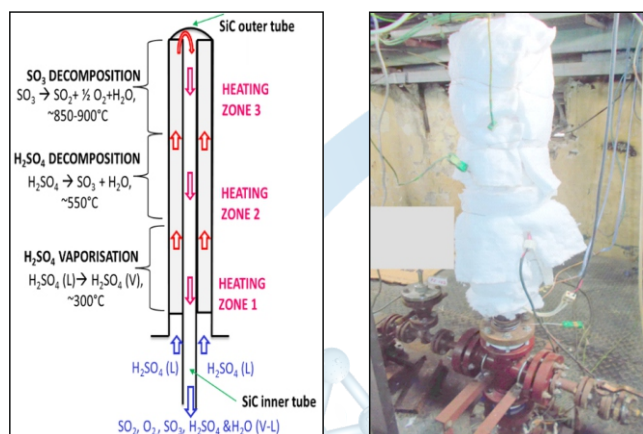


Fig. 7: Sulfuric acid decomposition scheme and experimental setup.



Fig. 8: HI decomposition setup.

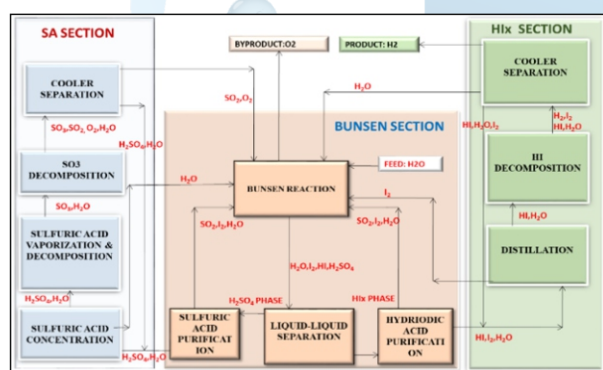


Fig. 9: Schematic of I-S process.

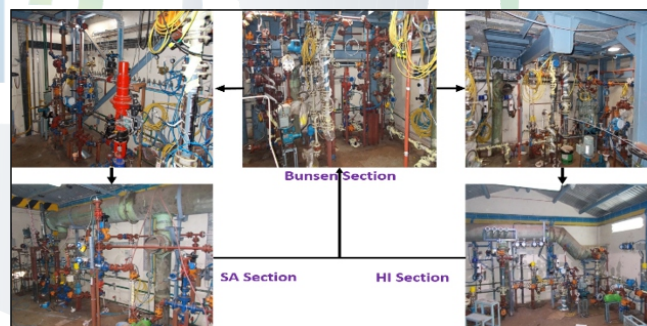


Fig. 10: Metallic closed loop I-S Process facility.

Subsequently, various process equipment and subsystems were fabricated, integrated, and tested under prototypical operating conditions, culminating in the successful demonstration of the complete I-S process in a closed-loop configuration. Based on the experience gained and performance demonstrated, a higher-scale I-S process facility is currently being established to advance the technology towards larger-scale operation. Further, modified configurations of the I-S process are envisaged for integration with HTGCR and, subsequently, for industrial deployment. These efforts will provide a systematic pathway for scaling up the technology and enable the eventual realization of the I-S process at an industrial scale for large-scale hydrogen production.

Acknowledgements

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हरित हाइड्रोजन उत्पादन के लिए भा.प.अ. केंद्र में निम्न तापमान वाली जल विद्युत अपघटक प्रौद्योगिकियों का विकास

Development of Low Temperature Water Electrolyser Technologies at BARC for Green Hydrogen Production

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सारांश

आयातित कच्चे तेल पर निर्भरता को कम करने, आयात व्यय को कम करने और दीर्घकालिक ऊर्जा सुरक्षा को बढ़ाने के लिए एक मजबूत हरित हाइड्रोजन अवसंरचना विकसित करना महत्वपूर्ण है। निम्न तापमान वाला जल विद्युत अपघटन हरित हाइड्रोजन उत्पादन के लिए एक आशाजनक उपाय है क्योंकि यह अक्षय ऊर्जा और नाभिकीय ऊर्जा सहित विभिन्न कार्बन मुक्त बिजली स्रोतों के साथ संगत है। यह बड़े पैमाने पर परिनियोजित आवश्यक लचीलापन और स्केल-क्षमता प्रदान करते हुए उच्च-शुद्धता वाले हाइड्रोजन के कुशल उत्पादन को सक्षम बनाता है। चूंकि औद्योगिक विद्युत अपघटक स्टैक मुख्य रूप से आयात किए जाते हैं, इसलिए आत्मनिर्भरता प्राप्त करने के लिए स्वदेशी प्रौद्योगिकी विकसित करना आवश्यक है। भारी पानी प्रभाग, भापअ केंद्र में क्षारीय जल विद्युत अपघटक प्रौद्योगिकी को 4 NL/h से बढ़ाकर लगभग 100 Nm³/h कर दिया गया है, जिसमें 10 Nm³/h प्रौद्योगिकी को एचपीसीएल, बीपीसीएल और बीएचईएल सहित 11 उद्योगों को हस्तांतरित किया गया है। स्वदेशी केशिका, संकर प्राकृतिक परिसंचरण और पीईएम जल विद्युत अपघटक भी सफलतापूर्वक विकसित किए गए हैं।

ABSTRACT

Developing a robust green hydrogen infrastructure is of strategic significance for the nation due to the high dependency on crude oil imports. Green hydrogen provides a sustainable pathway to reduce dependence on fossil fuels and to decarbonise the key industrial sectors including refineries and steel. Low-temperature water electrolysis is one of the most promising options due to its compatibility with variable load renewable energy sources such as solar power and continuous baseload nuclear power. As industrial electrolyser stacks are currently imported, at Heavy Water Division, BARC, alkaline water electrolyser technology has been developed indigenously and scaled up from laboratory-scale with hydrogen production capacity of 4 NL/h to industrial-scale systems of nearly 100 Nm³/h. The technology of 10 Nm³/h hydrogen production has been transferred to 11 industries, including HPCL, BPCL and BHEL. In addition, advanced capillary and hybrid natural circulation electrolyzers, as well as an indigenous lab scale PEM water electrolyser stack have also been successfully developed, demonstrating comprehensive national capability in advanced hydrogen production technologies.

KEYWORDS: Green hydrogen, Alkaline Water Electrolysis (AWE)



भा.प.अ. केंद्र में परीक्षण किए जा रहे प्रोटोटाइप 0.5 MW और 1 MW क्षारीय जल विद्युत अपघटक स्टैक ढेर।

Prototype 0.5 MW and 1 MW Alkaline water electrolyser stacks under testing at BARC

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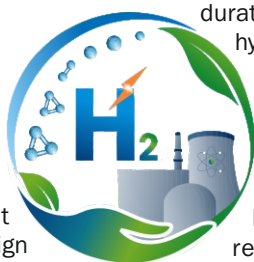


Introduction

Green hydrogen is emerging as a promising option for global decarbonization due to its potential to replace the fossil fuels in different industries including refineries, steel and fertilizer industries. Among the available hydrogen production methods, water electrolysis using renewable and nuclear energy offers a clean and sustainable route for hydrogen generation without carbon dioxide emission. The process involves electrochemical decomposition of water into oxygen and hydrogen with electricity as the source of energy. Various electrolyser technologies such as Alkaline Water Electrolysis (AWE), Proton Exchange Membrane Water Electrolysis (PEMWE), Solid Oxide Electrolysis Cells (SOEC), and Anion Exchange Membrane Water Electrolysis (AEMWE) have been explored globally with each process having specific advantages and limitations related to efficiency, operating conditions, and cost. However, large-scale deployment of electrolytic hydrogen production still faces challenges including high capital cost, catalyst and membrane durability, renewable energy intermittency, stack degradation, and lack of hydrogen storage and transportation infrastructure. Continued advancements in materials, stack design, and system integration are therefore essential for achieving the cost-effectiveness and sustainable green hydrogen production.

Low Temperature Water Electrolyser Technologies

Low-temperature water electrolyser technologies are gaining significant global attention for green hydrogen production due to their relatively simple operation and hydrogen production in a single step with high hydrogen purity at ambient conditions. The electrolysers are modular in design and its capability to work at large turn down ratio is also well known. Hence, electrolysers are considered as the most promising option for coupling with the renewable energy sources. The major low-temperature electrolyser technologies include Alkaline Water Electrolysis (AWE), Proton Exchange Membrane Water Electrolysis (PEMWE), and Anion Exchange Membrane Water Electrolysis (AEMWE). Among these, AWE is the most preferred option in terms of maturity, owing to its low cost, long operational life, and use of non-precious catalysts, although in general, it is limited from lower current density. PEMWE offers higher current density, compact system design, rapid response to fluctuating renewable power and high-pressure hydrogen production, but its deployment in industries is limited by high capital cost and dependence on expensive noble metal catalysts and membranes. AEMWE is a promising next-generation electrolyser technology that seeks to combine the benefits of conventional alkaline and PEM electrolysers by enabling the use of low-cost, non-precious metal catalysts within a compact cell architecture. However, subsequent improvements in membrane stability, ionic conductivity, and stable long-term operational performance are required before widespread commercialization. At present, alkaline and proton exchange membrane electrolysers constitute the largest share of the global installed electrolysis capacity, with their deployment accelerating in response to national hydrogen initiatives and worldwide decarbonization objectives.



Indian Scenario

In Indian context, establishing hydrogen infrastructure is critically important due to the country's large dependence on fossil fuel imports and the significant economic constraints associated with rising import bills. India imports a major portion of its fossil fuel requirement, making economy highly volatile due to the changes in oil prices globally, geopolitical conflicts, and supply chain disruptions. Therefore, critical national priorities will still remain as energy security and self-reliance. In this regard, green hydrogen offers a promising pathway for decreasing dependence on imported fossil fuels while supporting for a sustainable transition using indigenous technologies. India possesses significant potential for renewable energy generation owing to its large geographical area, high solar irradiance and extensive coastline. The country has abundant renewable energy resources that can be effectively utilized for large-scale green hydrogen production through water electrolysis. The electrolysers can be effectively integrated with both intermittent renewable energy sources such as solar as well as stable nuclear power facilitating for the production of green hydrogen without carbon emissions. Such renewable / nuclear-assisted electrolysis systems offer several advantages including reduction in greenhouse gas emissions, utilization of surplus renewable electricity, grid balancing, long-duration energy storage, and production of high-purity hydrogen without carbon emissions. Green hydrogen offers a critical role in decarbonizing several hard-to-abate industrial sectors including petroleum refining, fertilizer production, steel manufacturing, transportation, power generation, and chemical industries. Replacement of fossil-fuel-derived hydrogen with green hydrogen can substantially reduce carbon dioxide emissions and minimize environmental pollution and climate change impacts. Recognizing its strategic importance, India has launched the National Green Hydrogen Mission to promote domestic hydrogen production, electrolyser manufacturing, and supporting infrastructure development. Indigenous development of electrolyser and hydrogen technologies is expected to strengthen national energy security, reduce import dependency, support industrial growth, and accelerate the transition to a sustainable low-carbon economy.

Indigenous Alkaline Water Electrolyser Technology Development

At present, all the industrial electrolyser stacks in the country using low temperature water electrolyser technologies are imported. Indigenous development of low temperature water electrolyser technologies is critically important for achieving energy security, technological self-reliance, and large-scale deployment of green hydrogen production. Since AWE is presently the most mature and commercially viable technology for bulk hydrogen generation, development of domestic expertise in alkaline electrolyser design, stack engineering, electrode preparation, diaphragm fabrication, balance-of-plant systems, and manufacturing infrastructure can significantly reduce dependence on imported technologies and critical components. Indigenous technology development also enables cost reduction through localization



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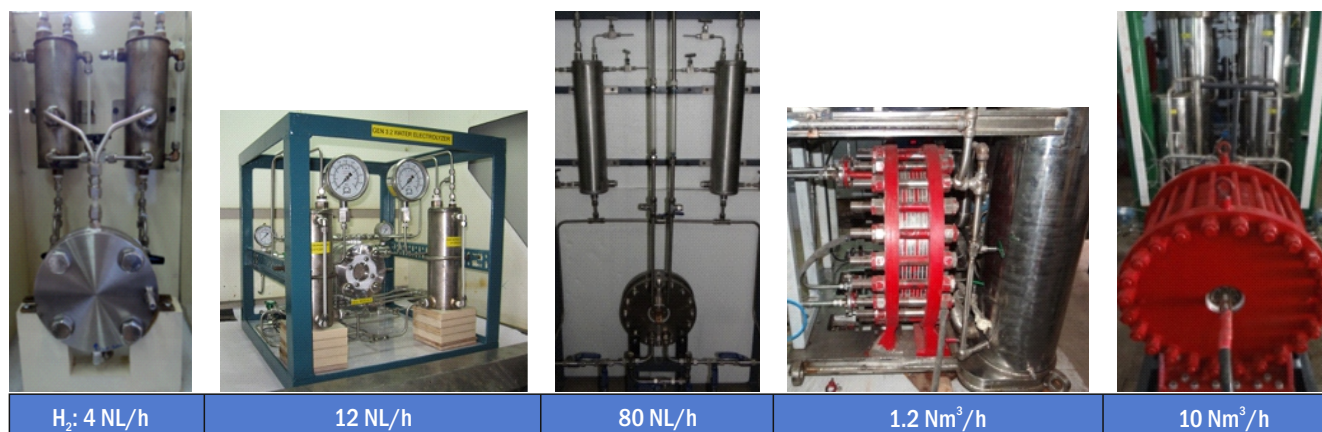


Fig.1: Different stages of development from 'lab to land'.

of materials and manufacturing, adaptation to Indian operating conditions, and creation of a robust domestic supply chain. Furthermore, it supports different industrial strategic sectors such as refineries, fertilizers, steel, heavy transport, and renewable energy storage while promoting national initiatives such as 'Make in India' and the 'National Green Hydrogen Mission'. Development of domestic alkaline electrolyser technology is also essential for enhancing long-term technological competitiveness, generating skilled employment, supporting export opportunities, and ensuring energy resilience against global supply chain disruptions and geopolitical uncertainties.

Based on the above vision, Heavy Water Division (HWD), BARC has initiated the indigenous development of both alkaline and PEM water electrolyser technologies from lab scale to industrial scale. The development of porous nickel electrodes constituted a key technological advancement in the alkaline water electrolyser development program undertaken at HWD, BARC [1]. This porous structure provides high surface area and improves electrochemical reaction rates, reduces overpotential, and increases hydrogen production efficiency. In addition, porous nickel electrodes facilitate efficient gas bubble release and mass transfer, making them highly suitable for high-current-density and large-scale alkaline water electrolysis applications. Nickel is selected as electrode material because of its favourable electrical conductivity, combined with adequate catalytic activity.

Different Developmental Stages of AWE Technology

The development of porous nickel electrode fabrication technology was initiated at the laboratory scale using electrodes of approximately 50 mm diameter. An alkaline water electrolyser stack of single cell with hydrogen production capacity of 4NL/h is designed and operated at a current density of 5000 A/m².

Subsequently, multi-cell bench-scale electrolyser systems were developed to investigate the influence of stacking configuration and electrolyte circulation on system performance. A three-cell stack electrolyser stack was fabricated and tested under similar operating conditions for hydrogen production rate of 12 NL/h. Based on the confidence gained from these studies, the electrode diameter was

progressively increased to three times for further scale-up investigations using larger two-cell stack configurations. In later stages, the electrode size was expanded up to ten times and the electrolyser modules were designed for operation at elevated pressures. A six-cell stack electrolyser capable of producing approximately 1.2 Nm³/h hydrogen was developed, with particular emphasis on electrolyte distribution and thermal management within the stack to ensure stable high current density operation. Subsequent scale-up efforts led to the development of a larger electrolyser system comprising two cell-module stacks arranged hydraulically in parallel and electrically in series, capable of producing 10 Nm³/h of hydrogen with an overall power requirement of approximately 50 kW. The integrated skid-mounted plant was also designed, which includes process systems for gas purification, pressure and flow regulation, gas-liquid separation, chilled water circulation, DC power supply and demineralized water feeding. The fully automated system is designed for continuous on-site hydrogen generation and delivery. The operation of the above plant has been carried out for more than 5000 hours. Four such units were developed and deployed at various sites. Subsequently, the indigenous alkaline water technology developed at BARC at a scale of 10 Nm³/h hydrogen production (50kW) has been transferred to 11 Indian industries. The different developmental phases from "lab to land" at HWD, BARC is shown in Fig.1.

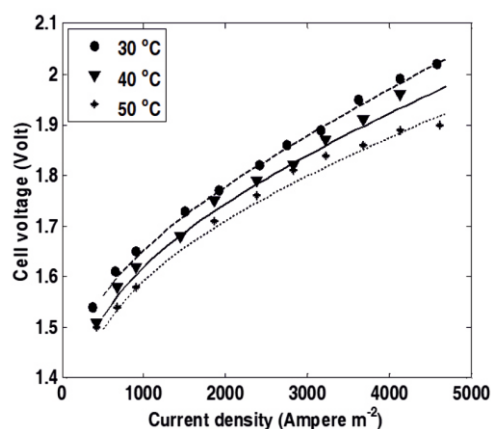


Fig.2: The polarization characteristics of the cell module stack at different temperatures [1-2].



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Table-1: Comparison of Ohmic parameter (Ωm^2) with literature [1-3].

Temperature (°C)	Ohmic parameter (Ωm^2)	
	Reported	BARC Electrolyser
30	7.3×10^{-5}	6.79×10^{-5}
40	7.05×10^{-5}	5.28×10^{-5}
50	6.8×10^{-5}	4.56×10^{-5}

Table-2: Lumped exchange current density parameter j_0 (A/m^2): Reported literature and present study [1-4].

Temperature (°C) ++	j_0 (A/m^2)	
	* Reported for Ni at 30% KOH	BARC Electrolyser
30	6.9540	12.0385
50	18.3251	43.8569
* Estimated based on the separate polarization data for anode and cathode		
++ Cathode parameters are reported in literature at 28 °C and 52 °C		

Electrochemical Performance of the Cell

The dependence of cell voltage on current density at different operating temperatures for the developed electrolyser cell module of 10 Nm³/h hydrogen generation plant is shown in Fig.2 [1-2]. The overall cell voltage is primarily influenced by Ohmic resistance and activation overpotential losses. The parameters governing different sources of performance loss can be estimated by evaluating the electrochemical polarization characteristics of the system. The Ohmic parameter, representing resistive losses within the cell, was evaluated and compared with values reported for electrolyzers available in literature (Table-1). The present indigenously developed BARC cell module exhibited comparatively lower resistance over the operating temperature range of 30–50 °C than the reported systems [3]. Compared with previously published studies, BARC developed electrolyser demonstrates reduced Ohmic resistance, indicating superior cell efficiency and overall performance. In addition, the exchange current density, which reflects electrode reaction kinetics and activation losses, was also analysed. Higher exchange current density values correspond to superior electrocatalytic activity of the electrode and lower activation overpotential. Comparison with literature data (Table-2) indicates improved electrode kinetics for the presently developed porous electrodes assembled in the cell module. Detailed electrochemical analysis is provided in Ref. [1-2]. The developed electrolyser achieved a current density of ~ 5000 A m⁻² at a cell voltage of ~1.9 V, even at a relatively low operating temperature of 50 °C compared to industrial stacks operating at >70 °C, demonstrating favourable electrochemical performance.



Industrial Collaborations

The indigenous alkaline water electrolyser technology developed at HWD, BARC, with 10 Nm³/h hydrogen production capacity, corresponding to power consumption of nearly 50kW, has been transferred to 11 Indian industries consists of leading Public Sector Units (PSU) such as BPCL, HPCL and BHEL and other key private industries including Bharat Forge, Godrej & Boyce and Thermax. The list of all alkaline water electrolyser technology transfer licensees is given in Fig.3 and all the licensees are at various stages of technology commercialization. HWD, BARC had also successfully incubated a 150 kW Alkaline water electrolyser technology through M/s Pratishna GreenTech, Mumbai and the developed system is shown in Fig.4. Due to the growing demand of green hydrogen, a need for scale up of the alkaline water electrolyser technology to MW scale was also initiated. HWD, BARC embarked on development of indigenous MW scale alkaline water electrolyser technology by developing 0.5 MW and 1 MW prototype stacks. The prototype stacks were tested successfully at BARC (Fig.5). Subsequently, a MoA has been formulated with BARC and BPCL for deployment of full scale 2 x 0.5 MW stacks for production of green hydrogen at the premises of Cochin International Airport (CIAL), Kochi. The full scale 0.5 MW stack was integrated with 1 MW Alkaline water electrolyser plant in collaboration with BPCL at the premises of CIAL, marking the world's first green hydrogen fuelling station in any airport premises [5]. The photograph of 0.5 MW indigenous electrolyser stack is shown in Fig.6.



Fig.3: List of 50 kW Alkaline Water Electrolyzer Technology Transfer Licensees.



Fig.4: 150 kW Alkaline water electrolyser plant developed under incubation.



Fig.5: Prototype 0.5 MW and 1 MW Alkaline water electrolyser stacks under testing at BARC.

Development of advanced passive alkaline water electrolyser stacks

Development of advanced passive alkaline water electrolyser stacks operating without external pumps for electrolyte recirculation are highly important for developing simple, rugged, energy-efficient and reliable hydrogen generation systems. In such systems, electrolyte circulation occurs naturally through density differences generated by gas evolution and temperature gradients within the electrolyser or by capillary forces, thereby eliminating the need for mechanical pumping systems. This significantly reduces auxiliary power consumption, maintenance requirements, operational complexity, and overall system cost. The absence of moving components also improves long-term reliability, minimizes vibration and leakage issues, and enhances safety during continuous operation. In addition, passive circulation systems offer compact design, lower balance-of-plant requirements and easier scalability, making them particularly attractive for decentralized and renewable energy-based green hydrogen production applications.

In HWD, BARC, the both the development of capillary electrolyser stack and natural circulation electrolyser stacks were also taken up. The capillary electrolyser represents an advanced alkaline water electrolysis technology capable of producing high-purity hydrogen and oxygen directly within the cell stack. As a result, it significantly reduces or eliminates the need for auxiliary Balance of Plant (BOP) systems that are



Fig.6: Indigenous 0.5 MW alkaline water electrolyser stack integrated with BOP in collaboration with BPCL at the premises of CIAL, Kochi.

conventionally employed for gas purification and conditioning. In capillary electrolysers, porous separator materials utilize capillary forces to sustain a thin electrolyte film on the electrode surface, facilitating electrochemical operation with minimal electrolyte inventory. A continuous supply of water is maintained at the electrochemically active sites, while the generated hydrogen and oxygen are efficiently evolved from the system, limiting gas bubble hold up and mitigating mass transfer limitations. Consequently, the design lowers Ohmic resistance, enhances the effective utilization of electrode surfaces, and supports energy-efficient hydrogen generation at elevated current densities. In this system, all the process components, except power supply and control system, are inbuilt in the cell module itself. A 10-cell stack of capillary electrolyser system is designed, fabricated and performance evaluation has been carried out meeting the design parameters. The photograph of 10 cell capillary scaled up stack is given in Fig.7.

In a natural circulation electrolyser, electrolyte circulation occurs due to density differences created by the evolution of hydrogen and oxygen gas bubbles during electrolysis. The gas-liquid mixture formed inside the cell rises upward, while comparatively denser electrolyte flows downward, establishing continuous circulation without the need for external pumps. This passive circulation mechanism improves heat removal, maintains electrolyte mixing, and reduces auxiliary power consumption and system complexity. The gas-liquid separator is provided as a part of internal construction feature in each half cell of the stack. A single cell stack of hybrid natural circulation electrolyser system (Fig.8) is



Fig. 7: Scaled up 10 Cell capillary electrolyser stack.



Fig.8: Hybrid natural circulation electrolyser stack under operation.



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Fig.9: Indegeneous PEM cell stack and PEM based laboratory hydrogen generator.

designed, installed and tested at a current density of 3000 A/m² with hydrogen production rate of ~40 NL/h while achieving a hydrogen purity of more than 99.9%. Further, a 10 cell stack has been designed and fabricated for 500 NL/h hydrogen gas production capacity.

PEM Water Electrolyser Technology Development

PEM water electrolyzers rely on ion-conducting polymer membranes and noble metal catalysts to efficiently drive electrochemical reactions. Noble metal catalysts are commonly utilized because of their excellent catalytic activity and long-term operational stability. A key advantage of this technology is its capability to produce high-purity, pressurized hydrogen directly from the electrolyser, thereby reducing the requirement for additional gas compression units. However, the dependence on expensive noble metals and specialized membrane materials can increase the overall system cost. In addition, PEM systems generally require highly purified water and careful operating conditions to maintain membrane durability and consistent performance over extended periods.

In alignment with the “Make in India” initiative and the goal of developing indigenous hydrogen generation technologies, HWD, BARC has successfully designed and fabricated a Membrane Electrode Assembly (MEA) based on Perfluoro-sulfonic acid (PFSA) membranes for PEM water electrolysis applications. The developed MEA was integrated into an in-house engineered electrolyser cell body, where it demonstrated stable operation at a current density of 10,000 A/m² with an operating voltage of approximately 1.9 V, exhibiting performance comparable to commercially available imported PEM electrolyzers. During the course of development, several technical challenges related to membrane-electrode integration, catalyst utilization, interfacial contact resistance, sealing integrity, and stable operation under high current density conditions were addressed through optimization of fabrication protocols and cell design. Particular emphasis was placed on achieving improved proton transport, uniform catalyst distribution, and enhanced mechanical stability to ensure reliable long-term operation. Subsequent evaluation of the fabricated PEM water electrolyzer single cell at room temperature, sustained and reliable operation for more than 1200 hours is carried out, delivering hydrogen at a rate of 10 NL/h with a dry basis purity of 99.99%. Subsequently an indigenous laboratory PEM based hydrogen generator with capacity of 18 NL/h is developed and completed operational trial runs of 500 hours. The photograph

of the system is shown in Fig.9. Building upon these successful demonstrations, ongoing efforts are focused on scaling up the system to a hydrogen generation capacity of 500 NL/h while further improving efficiency, durability, and operational reliability.

Conclusion

Low-temperature water electrolyser technologies play a major role in the large-scale generation of green hydrogen due to their operational simplicity, modular scale up and compatibility with renewable energy sources. Significant progress has been achieved at HWD, BARC through the indigenous development and scale-up of alkaline water electrolyzers, beginning from laboratory-scale of 4 NL/h hydrogen production capacity to industrial-scale systems of approximately 1 MW capacity (200 Nm³/hr). Performance evaluation of the developed electrolyser 50 kW stacks indicated superior electrochemical characteristics compared to reported literature data. Four such electrolyser plants of 10 Nm³/h capacity were successfully operated continuously for over 5000 hours and subsequently installed at user locations for field operation. The successful demonstration of the technology led to its commercialization through transfer to 11 industrial partners, including leading PSUs such as HPCL, BPCL and BHEL. In addition to conventional alkaline electrolyzers, advanced concepts such as capillary electrolyzers and hybrid natural circulation electrolyzers have also been developed to reduce auxiliary power consumption, and simplify system design with better energy efficiency. Furthermore, an indigenous PEM water electrolyser stack with a hydrogen generation capacity of 18 NL/h has been successfully developed, demonstrating the capability in advanced PEM water electrolyser technologies. These developments establish strong technological competence at BARC in electrolyser design, stack engineering, and hydrogen production systems, contributing significantly toward self-reliance and the advancement of the green hydrogen economy.

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नाभिकीय-संयुग्मित हाइड्रोजन उत्पादन हेतु कॉपर-क्लोरीन ऊष्मारासायनिक चक्र का विकास: भा.प.अ. केंद्र में विकास की स्थिति एवं भावी कार्य-योजना

Development of Copper-Chlorine Thermochemical Cycle for Nuclear Coupled Hydrogen Production: Developmental Status and Roadmap at BARC

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सारांश

नाभिकीय-संयुग्मित हाइड्रोजन उत्पादन की दिशा में प्रयास के अंतर्गत, भारत के भाभा परमाणु अनुसंधान (भा.प.अ.) केंद्र में कॉपर-क्लोरीन (Cu-Cl) ऊष्मारासायनिक चक्र का विकास व्यापक अनुसंधान एवं विकास (R&D) तथा समयबद्ध परिनियोजन हेतु अभियांत्रिकी गतिविधियों के माध्यम से सक्रिय रूप से किया जा रहा है। भा.प.अ. केंद्र में विकसित Cu-Cl चक्र की परिकल्पना बड़े पैमाने पर हाइड्रोजन उत्पादन के लिए की गई है। इस प्रौद्योगिकी की प्रमुख विशेषताओं में उच्च तापीय-से-हाइड्रोजन दक्षता, न्यूनतम सहायक चरणों एवं ठोस पदार्थ के प्रबंधन के साथ सघनित एकीकरण योजना तथा लगभग 500°C के मध्यम तापमान की आवश्यकता सम्मिलित है। ये विशेषताएँ इसे मध्यम एवं उच्च तापमान वाले नाभिकीय रिएक्टरों के साथ संयोजन हेतु अत्यंत संभावनाशील बनाती हैं। विकास संबंधी प्रयासों के परिणामस्वरूप, भा.प.अ. केंद्र की Cu-Cl प्रौद्योगिकी ने कई महत्वपूर्ण उपलब्धियाँ प्राप्त की हैं। इस प्रौद्योगिकी का बेंच-स्केल पर 5 NL/h हाइड्रोजन उत्पादन दर पर 170 घंटे की सतत अवधि तक सफल प्रदर्शन किया गया है, जो विश्व स्तर पर किसी भी ऊष्मारासायनिक चक्र के लिए अब तक प्रतिवेदित सर्वाधिक अवधि का संचालन है।

ABSTRACT

In a quest for nuclear coupled hydrogen production, the development of Copper-Chlorine (Cu-Cl) thermochemical cycle is being actively pursued at Bhabha Atomic Research Center (BARC), India through extensive R&D and engineering for time bound deployment. The Cu-Cl cycle developed at BARC is envisaged for large scale hydrogen production encompassing several salient features which includes high thermal to hydrogen efficiency, an intensified integration scheme with minimal auxiliary steps and solid handling and moderate temperature requirement of around 500°C, which renders it eminently prospective for coupling with moderate and high temperature nuclear reactors. As an outcome of the developmental endeavors, the Cu-Cl technology of BARC has achieved significant milestones. The technology has been demonstrated at bench-scale at 5 NL/h hydrogen throughput for a sustained duration of 170 hours, making it the highest reported operation for any thermochemical cycle globally. Subsequently, a pilot-scale facility of design capacity 150 NL/h hydrogen throughput has been commissioned and demonstrated for 220 hours. The present article discloses all the developmental milestones and future roadmap pertaining to Cu-Cl thermochemical technology of BARC for expedited deployment of nuclear hydrogen production.

KEYWORDS: *Copper-Chlorine, Cu-Cl, Nuclear, Hydrogen, Thermochemical cycle, Pilot-scale*



एकीकृत क्यू-सी. एल.-एफ. बी. टी. आर. सुविधा

Integrated Cu-Cl-FBTR facility

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Introduction

The onset of the hydrogen ecosystem in the last decade has propelled innovations and cutting-edge research towards development of state-of-the-art hydrogen production technologies. In particular, nuclear coupled hydrogen production offers distinctive advantages which include large scale production capability, high availability factor, captive and non-captive production philosophy and low levelized cost of hydrogen. In line with the objective of manifesting nuclear hydrogen production, a distinctive class of hydrogen production technology viz. thermochemical cycles are being developed globally. The thermochemical cycles achieve water splitting using a series of chemical reactions carried out in a closed loop, resulting in a net output of hydrogen and oxygen with complete recycle of all intermediate chemicals.

Development of Cu-Cl thermochemical cycle is being actively pursued at BARC in a staged sequential approach comprising of key milestones for time bound deployment of the technology. The initial phase encompassed establishing the feasibility of constituent steps, reaction mechanism and kinetics, modelling of multiphase reactors and development of auxiliary sub-systems for achieving integration of the loop, as reported by Thomas et al. [1-4]. Following this, activities pertaining to demonstration of integrated bench-scale facility were undertaken, encompassing development of a novel integration scheme for closed loop operations, control and instrumentation heuristics, detailed engineering activities and MOC development for key components. As an outcome of the developmental endeavours, a first of its kind bench-scale facility, as illustrated in Fig.1, corresponding to a TRL of 5 was demonstrated at 5 NL/h hydrogen production for a sustained duration of 170 hours, making it the highest recorded duration for any thermochemical cycle globally [5-6]. Subsequently, based on design and operational feedback from the bench-scale facility, a pilot facility (TRL-6) was installed and commissioned with a design capacity of 150 NL/h H_2 , as illustrated in Fig.2. The facility has been demonstrated at 150 NL/h for 220 hours thereby establishing the design basis and integration scheme. The pilot-scale facility encompasses several state-of-the-art systems for multiphase thermal steps, novel separation processes, non-mechanical high temperature solid handling, control and instrumentation. In view of the developments an application has been filed with the Indian Patent Office towards grant of intellectual property (IP) rights.

Nuclear Hydrogen

As part of the expedited initiative to establish the feasibility of coupling Cu-Cl cycle with nuclear reactors of Department of Atomic Energy, several endeavours have been undertaken. The focus is towards coupling with two high temperature reactors viz. Fast Breeder Reactors, in particular FBTR and secondly the upcoming High Temperature Gas Cooled Reactor (HTGCR). Dedicated activities on multiple fronts have been initiated towards achieving these targets, which involves several first of its kind developments towards establishing the coupling philosophy. This section discusses in detail the pertinent activities.

Coupling with Fast Breeder Reactors

Chemical Engineering Division (ChED) of BARC in coordination with IGCAR have embarked upon activities to couple the pilot-scale Cu-Cl facility with secondary sodium loop of FBTR, for demonstration of nuclear H_2 production. The main objective of this demonstration is to establish the feasibility of coupling the Cu-Cl process, most primarily the two thermal reactors viz. hydrolysis and thermolysis with sodium systems. The pilot-scale facility has suitably been re-engineered for this purpose. The process and thermal hydraulic design have been carried out for the thermal reactors, with objective to facilitate extraction of heat from secondary sodium loop of FBTR. Further, several key developments, which include safe thermal reactor design, fast acting safety systems, control philosophy and detailed analysis of safety scenarios have been carried out. The Cu-Cl pilot scale facility at BARC was dismantled, transported and re-installed at FBTR, IGCAR. Several new technical systems were also designed and installed to facilitate the coupling interface. At present, the facility has been installed and coupled with secondary sodium loop of FBTR as illustrated in Fig 3.

The coupled pre-commissioning activities and cold-commissioning have been completed. During pre-commissioning, the performance of all the critical engineered systems including the process design of thermal reactor was established as per design intent. Subsequently, the commissioning and demonstration of nuclear hydrogen was carried out as per design capacity on 26th June, 2026. The campaign established operation of the integrated facility and performance of all systems as per design intent. No anomalies in operation and safety were observed during the campaign. This demonstration of Cu-Cl facility coupled with FBTR marks the first instance of hydrogen production using nuclear heat in the world. The facility will act as a test-bench and will be used for generating critical engineering data which will be required for further scale-up and deployment of Copper-Chlorine technology coupled with sodium cooled fast reactors. Additionally, design and associated pre-project activities have been initiated for a future scaled-up Copper-Chlorine facility coupled with upcoming FBTR-II. The design and detailed engineering of the facility pertinent to the hydrogen production process is being carried out by ChED, BARC.



Fig.1: Integrated novel bench-scale facility in metallic systems.



Fig.2: Integrated novel pilot-scale facility in metallic systems.

Prototype Facility

As a major target of Department of Atomic Energy, the Copper-Chlorine cycle is being designed and scaled-up for coupling with the upcoming gas cooled reactors. The gas coolant from the reactors will be utilized to drive the thermal reaction steps. Since, this being a first of its kind project in the world, there is no precedence and previous engineering data available for such systems. In view of this, a prototype Copper-Chlorine facility with a design capacity of $10 \text{ Nm}^3/\text{h}$ ($\sim 1 \text{ kg/h}$) is being installed at BARC. The facility will encompass a simulated high temperature gas loop integrated with the Copper-Chlorine process systems. The facility is being designed with an objective to serve as the miniaturized version of the Copper-Chlorine technology which will be deployed. The facility constitutes of novel design of chemical reactors, especially the thermal reactors with extended surfaces, intensified process systems and highly efficient internal heat recovery systems comprising of direct contact heat exchangers and multi-phase heat exchangers having optimized geometry to achieve maximum possible heat recovery, thereby enhancing the overall efficiency of the Copper-Chlorine cycle. The prototype facility will have a technology readiness level (TRL) of 8-9, which will make it ready for deployment. The detailed design of the facility has been completed and the tendering and installation activities are in progress. The facility will provide critical engineering data and will be used for establishing the performance of scaled-up systems and other critical engineering systems of Copper-Chlorine technology.

Demonstration Facility Coupled with Gas Cooled Reactor

As part of one of the major commitments under the aegis of Nuclear Energy Mission, 2025 by the Government of India, a large-scale demonstration facility is being set-up at BARC, Vishakhapatnam. The upcoming facility will be a large-scale centralized facility dedicated entirely for nuclear hydrogen production. The Copper-Chlorine facility will be coupled with the upcoming 5MWth high temperature gas cooled reactor (HTGCR) as the heat source for the Copper-Chlorine process, a first of its kind dedicated project in the world. The design and engineering of the facility have been completed and the associated pre-project activities are underway. The key highlights of the Copper-Chlorine facility include novel design of thermal reactors with extended surfaces to extract maximum heat utilization from the nuclear coolant, intensified process systems and highly efficient internal heat recovery systems. The major highlight of the upcoming facility is its



Fig.3: Integrated Cu-Cl-FBTR facility.

completely indigenous designed and developed process systems. The upcoming facility at Vizag will offer end-to-end solution for hydrogen and will act as a well to gate technology demonstrator for nuclear hydrogen production.

Conclusion

BARC has demonstrated the first of its kind Copper-Chlorine (Cu-Cl) thermochemical cycle for production of clean hydrogen through water splitting using a series of closed loop chemical reactions. Further scale-up and deployment activities are being pursued in mission mode and directed towards technology demonstration with prospective high temperature reactors for hydrogen production using nuclear power. By leveraging cleaner nuclear power, the developmental efforts aim to establish a reliable and sustainable method of hydrogen production, leading to self-reliance/Aatmanirbharta in energy security. Also, the project aligns with India's ambitious Net Zero directives set under 'Nuclear Energy Mission'.

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हाइड्रोजन उत्पादन के लिए उच्च-तापमान वाष्प विद्युत अपघटन

High-Temperature Steam Electrolysis for Hydrogen Production

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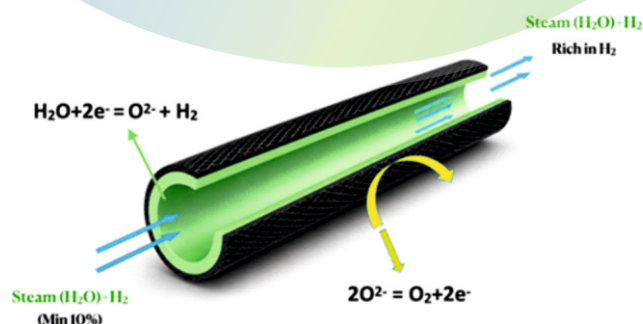
सारांश

ऊर्जा सुरक्षा, जीवाश्म ईंधन की कमी और हरित गृह गैस उत्सर्जन पर बढ़ती चिंताओं ने दीर्घकालिक हाइड्रोजन उत्पादन में रुचि बढ़ा दी है। ठोस ऑक्साइड विद्युत अपघटन सेलों (एसओईसी) का उपयोग करके उच्च तापमान वाले भाप विद्युत अपघटन (एचटीएसई) हाइड्रोजन उत्पादन के लिए सर्वाधिक ऊर्जा-कुशल तरीकों में से एक है। उत्थापित तापमान पर प्रचालन करते हुए, एचटीएसई वाष्प-विभाजन आवश्यकता के हिस्से की आपूर्ति के लिए तापीय ऊर्जा का उपयोग करता है, बिजली की खपत को कम करता है और कम तापमान वाले विद्युत अपघटन की तुलना में दक्षता में सुधार करता है। प्रौद्योगिकी को बड़े पैमाने पर हाइड्रोजन उत्पादन के लिए प्रगत परमाणु रिएक्टरों, केंद्रित सौर ताप प्रणालियों और औद्योगिक अपशिष्ट ऊष्मा स्रोतों के साथ प्रभावी ढंग से एकीकृत किया जा सकता है। भाभा परमाणु अनुसंधान केंद्र (बीएआरसी) में महत्वपूर्ण अनुसंधान एवं विकास प्रयासों ने ट्यूबलर एचटीएसई प्रौद्योगिकी पर ध्यान केंद्रित किया है। ट्यूबलर एसओईसी के लिए स्वदेशी विनिर्माण प्रौद्योगिकी को सफलतापूर्वक विकसित किया गया है, और 800 °C पर 150 घंटे से अधिक समय तक स्थिर प्रचालन का प्रदर्शन किया गया है, जिससे 4 NL h⁻¹ की औसत हाइड्रोजन उत्पादन दर प्राप्त हुई है। यह शोध पत्र एचटीएसई प्रौद्योगिकी की समीक्षा करता है, जिसमें प्रचालनीय सिद्धांतों, पदार्थों, स्टैक विन्यास और ट्यूबलर एसओईसी विकास में चुनौतियों पर ज़ोर दिया गया है।

ABSTRACT

Growing concerns over energy security, fossil fuel depletion, and greenhouse gas emissions have accelerated global interest in sustainable hydrogen production technologies. Hydrogen is widely regarded as a clean energy carrier because its utilization generates only water, making it a promising option for decarbonization of the energy and industrial sectors. However, most of the hydrogen currently produced worldwide is derived from fossil-fuel-based processes which are associated with considerable CO₂ emissions. Among various low-carbon hydrogen production routes, high-temperature steam electrolysis (HTSE) employing solid oxide electrolysis cells (SOECs) has emerged as one of the most energy-efficient electrochemical routes for hydrogen generation. HTSE operates at high temperatures, allowing part of the energy required for steam splitting to be supplied as heat instead of electricity. The favourable thermodynamics and faster electrochemical reactions at high temperatures reduce the electrical energy required for HTSE compared with low-temperature electrolysis systems. Furthermore, HTSE can be effectively integrated with advanced nuclear reactors, concentrated solar thermal systems, and industrial waste-heat sources for large-scale hydrogen production. R&D activities on tubular HTSE technology for hydrogen production applications have been undertaken at Bhabha Atomic Research Centre. Fabrication technology for tubular HTSE cells has been successfully developed, and stable long-term operation of tubular cells has been demonstrated for more than 150 h at 800°C, achieving an average hydrogen production rate of 4 NL h⁻¹. This paper reviews HTSE technology, focusing on operating principles, thermodynamic benefits, materials selection, stack configurations, and key challenges in tubular HTSE development.

KEYWORDS: HTSE; SOEC; Tubular electrolysis cells; Nuclear-coupled hydrogen production; Hydrogen energy



ट्यूबलर उच्च तापमान वाष्प विद्युत अपघटन
(एचटीएसई) सेल का चित्र।

A schematic of a tubular HTSE cell

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Introduction

Hydrogen has emerged as a promising zero-emission energy carrier capable of facilitating the global transition to clean energy. It offers several advantages, including high gravimetric energy density, long-term energy security, and the ability to mitigate the intermittency of renewable energy sources [1]. Fig.1 illustrates an integrated HTSE-SOFC hydrogen energy cycle. The process begins with green hydrogen production via steam electrolysis utilizing thermal and electrical energy derived from nuclear or concentrated solar power. The generated hydrogen can be stored in gaseous, liquid, or solid-state forms such as metal hydrides, which provide high storage density and improved safety. Stored hydrogen can later be utilized in fuel cells for the direct generation of electricity with high conversion efficiency and near-zero pollutant emissions. During fuel-cell operation, water or steam is produced as a by-product, thereby completing a sustainable hydrogen cycle. The integration of hydrogen production, storage, and utilization technologies is considered a key strategy for the development of future low-carbon energy infrastructures and sustainable energy systems.

Global hydrogen demand reached nearly 100 million tonnes in 2024, with the majority of hydrogen currently produced from fossil fuels, primarily through steam methane reforming (SMR). Conventional hydrogen production routes are associated with substantial greenhouse gas emissions, contributing approximately 900–1000 Mt CO₂-equivalent emissions annually. Despite increasing global emphasis on clean energy transition pathways, less than 1% of global hydrogen production presently originates from low-emission routes such as water electrolysis using renewable or nuclear electricity [2,3].

Among the available hydrogen production technologies, alkaline (ALK) and proton-exchange membrane (PEM) electrolysis are the most commercially mature. However, these systems operate at relatively low temperatures (20–80°C) and

require high electrical energy input, with typical specific energy consumption in the range of 50–55 kWh kg⁻¹ of H₂ produced [2–4]. In contrast, HTSE based on SOECs operates at 700–850°C, where part of the energy required for water splitting is supplied as heat instead of electricity. From a thermodynamic perspective, the enthalpy change (ΔH) for water splitting remains relatively constant at approximately 242–250 kJ mol⁻¹ over the HTSE operating range, whereas the Gibbs free energy change (ΔG), representing the minimum electrical work required for electrolysis, decreases significantly with increasing temperature. At 25°C, ΔG is approximately 237 kJ mol⁻¹, while at 800°C it decreases to nearly 180–190 kJ mol⁻¹. As a result, more energy can be supplied as heat, reducing the electrical energy requirement [4,5].

The thermodynamic advantage of HTSE is manifested through reduced operating cell voltage and lower electrical power consumption. The thermoneutral voltage decreases from approximately 1.48 V at room temperature to nearly 1.29–1.30 V at 800°C. As a result, HTSE systems require approximately 25–35% less electrical energy than conventional low-temperature electrolysis technologies [4]. When coupled with high-temperature heat sources such as advanced nuclear reactors or solar thermal systems, HTSE can achieve thermal-to-hydrogen efficiencies of 45–59% on a lower heating value (LHV) basis, making it a promising technology for large-scale low-carbon hydrogen production [5].

The Department of Atomic Energy (DAE) is pursuing R&D programs focused on the development of advanced high-temperature nuclear reactor technologies [6]. Integration of HTSE with advanced high-temperature reactor systems has the potential to expand the application of nuclear energy beyond electricity generation to efficient large-scale hydrogen production. The hydrogen generated through HTSE can be utilized in long-term energy storage and synthetic fuel production pathways, thereby supporting sustainable low-carbon energy systems.

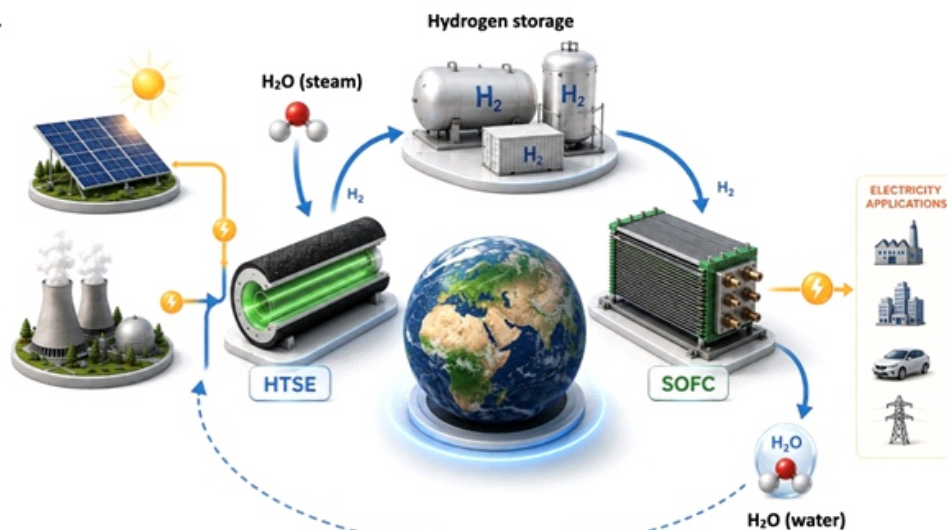


Fig.1: Schematic representation of an integrated HTSE-SOFC hydrogen energy cycle powered by renewable and nuclear energy sources.



Historical Development of HTSE Technology

The development of HTSE technology originated from early investigations on oxygen-ion-conducting ceramic electrolytes during 1960s. The development of stabilized zirconia electrolytes, particularly yttria-stabilized zirconia (YSZ), enabled operation above 800°C due to their high ionic conductivity and laid the foundation for SOFC and SOEC technologies. The global oil crisis of 1970s accelerated worldwide research on alternative energy technologies, including high-temperature electrochemical systems. During the late 1970s and 1980s, Westinghouse Electric Corporation pioneered the development of tubular SOFC architectures for elevated-temperature operation. The tubular configuration offered improved thermal shock resistance, simplified sealing requirements, and enhanced mechanical reliability, which later facilitated its adaptation for HTSE applications. Interest in HTSE increased after the 1990s because of growing focus on the hydrogen economy, renewable energy integration, nuclear-assisted hydrogen production, and decarbonization. Current research is focused on large-scale hydrogen production, reversible SOFC/SOEC systems, degradation mitigation, and integration with advanced nuclear reactors and renewable energy systems for efficient low-carbon hydrogen generation.

Operating Principles of SOFC and HTSE

SOFCs and HTSE systems operate through oxygen-ion transport across a dense ceramic electrolyte at 700–850°C. Both technologies employ similar cell architectures consisting of a porous fuel electrode, a dense oxygen-ion-conducting electrolyte, and an oxygen electrode, and are therefore considered reversible electrochemical systems. Fig.2 illustrates the operating principles of SOFCs and HTSE systems. In solid oxide fuel cell (SOFC) mode, chemical energy stored in fuels such as hydrogen is directly converted into electrical energy through electrochemical oxidation reactions. At the oxygen electrode, molecular oxygen undergoes electrochemical reduction to form oxygen ions, which subsequently migrate through the electrolyte toward the fuel electrode. At the fuel electrode, H₂

reacts with oxygen ions to produce steam while releasing electrons to the external circuit, thereby generating electrical power and heat.

In contrast, HTSE represents the reverse electrochemical operation of an SOFC. Instead of generating electricity, HTSE utilizes electrical energy and high-temperature steam to produce hydrogen through electrochemical steam reduction. At the steam/fuel electrode, steam undergoes electrochemical reduction to generate hydrogen and oxygen ions, while the oxygen ions migrate through the electrolyte toward the oxygen electrode, where oxygen evolution takes place. The electrolyte therefore serves both as an oxygen-ion conductor and as a gas-tight separator between the two electrode compartments. High operating temperatures improve reaction kinetics and oxygen-ion conductivity, reducing polarization losses and electrical power consumption.

Cell and Stack Geometries

HTSE systems are mainly classified into planar and tubular configurations (Fig.3), and the cell geometry strongly affects performance, thermal management, sealing, and durability. The planar geometry may be either electrolyte-supported, in which the electrolyte is thicker than the electrode layers, or electrode-supported, where one of the porous electrodes provides mechanical support for a thin electrolyte layer. Planar SOECs consist of flat multilayer ceramic cells assembled into stacks using metallic interconnects and high-temperature sealants. Their compact geometry provides high active-area utilization, short current collection paths, high volumetric efficiency, high power density, and reduced ohmic losses. Planar architectures are also well suited for large-area cell fabrication and scalable stack integration. However, these systems require complex high-temperature sealing arrangements and are more susceptible to thermo-mechanical stresses during operation and thermal cycling. The flat ceramic geometry further increases the risk of mechanical failure and gas leakage at sealing interfaces during prolonged high-temperature operation.

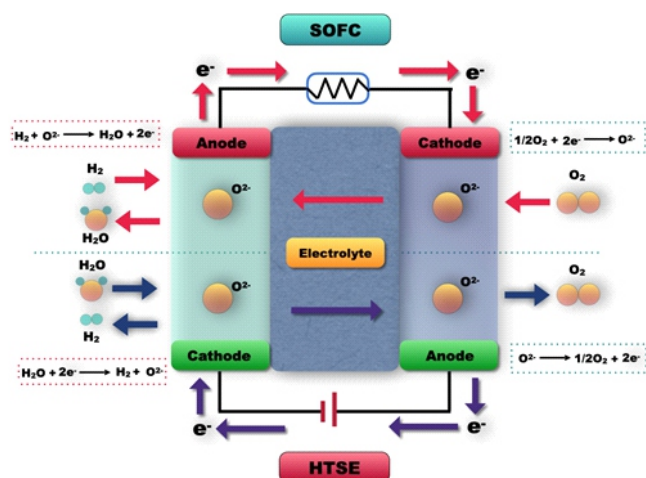


Fig.2: Schematic illustration of the operating principles of SOFC and HTSE, showing oxygen ion transport, electrode reactions, and electron flow during fuel cell and electrolysis modes.

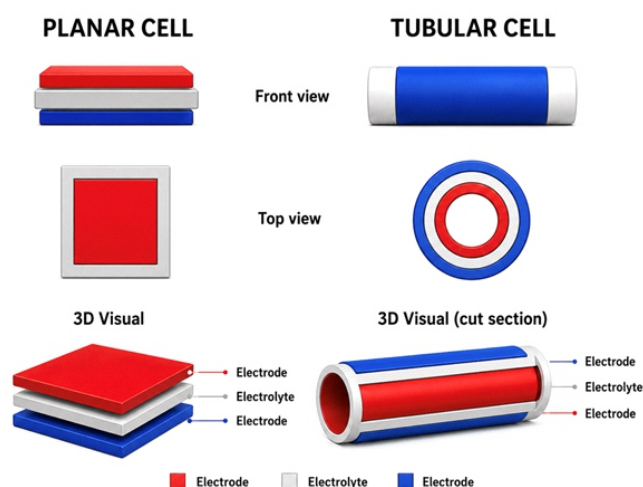


Fig.3: Schematic comparison of planar and tubular solid oxide cell configurations

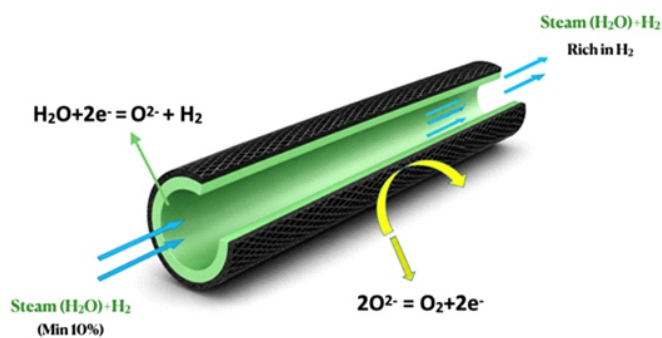


Fig.4: A schematic of a tubular HTSE cell.

Tubular HTSE cells comprise of cylindrical electrochemical structures in which electrode and electrolyte layers are concentrically deposited onto a tubular support. In the tubular configuration, one of the porous electrodes serves as the mechanical support tube on which a thin dense electrolyte layer is deposited, followed by deposition of the second porous electrode. Originally developed for tubular solid oxide fuel cells (SOFCs), this design was subsequently adapted for steam electrolysis applications. Tubular architectures offer superior thermal shock resistance, improved tolerance to thermal gradients and thermal cycling, simplified sealing requirements, and enhanced mechanical robustness. The tubular geometry reduces thermo-mechanical stress and gas leakage because fewer sealing joints are needed. These characteristics make tubular SOEC systems attractive for long-duration operation under harsh thermal environments and for nuclear-coupled HTSE applications requiring high thermal reliability. However, tubular HTSEs generally show lower power density and higher ohmic losses than planar designs because of longer current paths.

Components of Tubular HTSE and its Working Principle

HTSE is an all-solid-state electrochemical system in which both electrodes and the electrolyte are manufactured from ceramic-based materials. The most widely used electrolyte material for HTSE applications is yttria-stabilized zirconia (YSZ), owing to its excellent thermo-chemical stability and long-term operational reliability at elevated temperatures. The oxygen electrode is typically a perovskite oxide based on strontium-doped lanthanum manganite (LSM), whereas the fuel electrode generally consists of a porous Ni-YSZ cermet that provides both catalytic activity and electronic conductivity. HTSE stacks also require interconnects for electrical connection and high-temperature sealants for gas-tight operation. Interconnects are used for current collection and electrical connection between adjacent cells, while high-temperature sealants ensure hermetic separation between the fuel and oxygen compartments during prolonged high-temperature operation. The electrolyte layer must remain fully dense to prevent gas leakage and intermixing, whereas both electrode layers generally exhibit porosity in the range of 30–40 vol.% to facilitate gas transport and electrochemical reactions. The schematic of a tubular HTSE cell is shown in Fig.4. The tube is typically fabricated from porous NiO-YSZ material, over which a thin dense YSZ electrolyte layer is deposited, followed by coating of the Sr-doped lanthanum manganate (LSM) oxygen electrode. A mixture of steam and hydrogen is supplied to the fuel-electrode compartment of the tubular cell. A small amount of hydrogen (~10 vol.%) is added to maintain reducing conditions and prevent oxidation of the nickel electrode. During operation, a potential is applied between the two electrodes. At the fuel electrode, steam undergoes electrochemical reduction to generate hydrogen and oxygen ions. The oxygen ions are

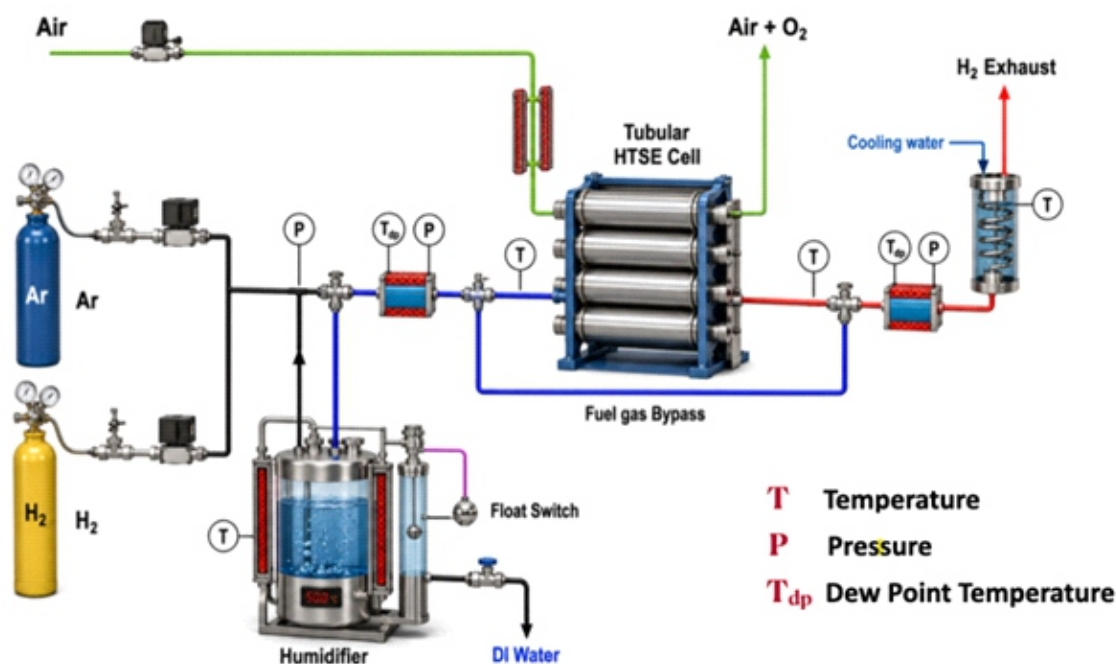


Fig.5: A schematic representation of test facility for electrochemical performance characterization of tubular HTSE cells.



Fig.6: Single Cell Tubular HTSE during long-term testing.

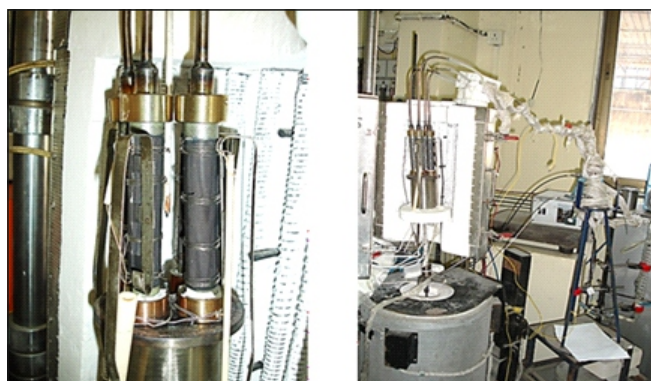


Fig.7: Multi-cell tubular HTSE assembly and testing.

subsequently transported through the dense oxygen-ion-conducting electrolyte under an applied electrical potential and are oxidized at the oxygen electrode to form molecular oxygen. During continuous electrolysis operation, hydrogen concentration within the fuel-electrode compartment progressively increases, while the outlet stream typically contains hydrogen together with unreacted steam. In HTSE operation, complete steam conversion is generally avoided to prevent steam starvation, electrode degradation, and concentration polarization. Consequently, downstream steam condensation or gas-separation processes are generally required to obtain high-purity hydrogen. Other important considerations in tubular HTSE systems include the long-term stability of sealants, electrical contact materials, and electrode-electrolyte interfaces under severe elevated-temperature redox conditions.



Current Status of HTSE development at BARC

At Bhabha Atomic Research Centre (BARC), fabrication technology for tubular HTSE cells has been successfully developed. A dedicated experimental facility for electrochemical performance characterization of tubular HTSE cells has been established [7]. A schematic representation of the test setup is shown in Fig.5. Using this facility, several long-term electrochemical performance studies of tubular HTSE cells were conducted. Under laboratory operating conditions, several tubular HTSE cells were operated continuously for 150 h at a current density of approximately 0.15 A cm^{-2} , corresponding to an average hydrogen production rate of about 4 NL h^{-1} (Fig.6). Electrochemical studies were conducted to evaluate the effects of temperature, steam flow rate, gas composition, electrical contact characteristics, and current density on hydrogen production [8,9]. To enhance the electrochemical performance of the tubular cell, the influence of various operating and process parameters on hydrogen production characteristics was systematically investigated through current density measurements. By optimizing the operating parameters, the tubular HTSE cells achieved a current density of 0.3 A cm^{-2} , which is generally considered a benchmark performance level for tubular HTSE systems reported in the literature. The studies showed that reducing interfacial and contact resistance is essential for improving hydrogen production and electrochemical efficiency. The investigations also indicated that electrical contact

degradation and thermo-mechanical instability at electrode-interconnect interfaces constitute important factors affecting long-term operational stability. Accordingly, ongoing research and development activities are focused on optimizing the electrical contact characteristics and interfacial stability of the cell components.

Following the successful demonstration of single tubular HTSE cell, fabrication and assembly of a four-cell tubular HTSE stack were undertaken. Fig.7 illustrates 4-cell HTSE Test assembly during electrochemical characterisation.

Preliminary long-term performance evaluations of the four-cell stack have shown encouraging results, while extended durability studies are currently in progress.

High-temperature glass sealants remain a major challenge because they must maintain sealing integrity, thermo-mechanical compatibility, and chemical stability under severe redox conditions.

Therefore, efforts were initiated toward the development of indigenous glass sealant materials suitable for HTSE and solid oxide fuel cell (SOFC) applications. Recently, an indigenous high-temperature glass sealant composition was successfully developed and evaluated under HTSE operating conditions. Long-term testing exceeding 300 h demonstrated satisfactory thermo-mechanical stability, chemical compatibility, and sealing integrity, indicating the suitability of the developed sealant for prolonged high-temperature operation.

Recent Developments in Nuclear-Coupled HTSE Systems

Recent studies have shown that hybrid nuclear-renewable-HTSE systems can improve grid stability and support flexible hydrogen production during periods of excess renewable power generation. Advanced reactor concepts, including High-Temperature Gas-Cooled Reactors (HTGRs), Small Modular Reactors (SMRs), molten salt reactors, and supercritical CO-cooled fast reactors, are being actively investigated for integrated hydrogen production applications. Thermodynamic analyses indicate that nuclear-assisted HTSE systems can achieve thermal-to-hydrogen efficiencies exceeding 50% under optimized operating conditions. Furthermore, optimized thermal integration, steam management, and waste heat recovery systems can further enhance overall plant efficiency and operational flexibility.



Recent studies have also demonstrated that hybrid nuclear-renewable-HTSE systems can improve grid stability and enable flexible hydrogen production during periods of excess renewable electricity generation [10-11]. Such hybrid systems offer promising solutions for seasonal energy storage and decarbonization of hard-to-abate industries.

Conclusions

Tubular HTSE represents a highly promising pathway for efficient and clean hydrogen production. Compared with conventional low-temperature electrolysis technologies, HTSE offers significantly higher thermodynamic efficiency because a substantial fraction of the energy required for steam splitting is supplied in the form of heat, thereby reducing electrical energy consumption. Tubular HTSE systems also offer advantages such as improved thermo-mechanical reliability, simpler sealing, better thermal cycling resistance, and higher structural stability. These characteristics make tubular HTSE systems attractive for integration with advanced nuclear reactors and renewable-energy-driven thermal systems.

India possesses substantial long-term strategic potential in nuclear-assisted hydrogen production because of its well-established nuclear energy programme, expertise in fast breeder reactor technology, and ongoing development of thorium-based nuclear systems. Integration of high-temperature nuclear reactors with tubular HTSE systems could enable large-scale green hydrogen production with low carbon emissions and support national energy security goals.

Developmental activities on tubular HTSE technology were initiated at Bhabha Atomic Research Centre, where fabrication technology for tubular HTSE cells has been successfully established. Stable long-term operation of a single tubular HTSE cell was demonstrated for more than 150 h at an operating temperature of 800°C, achieving an average hydrogen production rate of approximately 4 NL h⁻¹. In addition, development and long-term evaluation of a multi-cell tubular HTSE stack are currently in progress, with preliminary results indicating encouraging electrochemical performance and operational stability.

From the perspective of large-scale commercialization, further advances are required in the development of degradation-resistant electrode and interconnect materials, protective coatings against chromium volatilization, high-reliability sealing technologies, scalable ceramic manufacturing routes, and integrated thermal management strategies. Further research is required to mitigate long-term degradation caused by electrode delamination, nickel coarsening, chromium poisoning, redox instability, and thermal stress-induced cracking. Continued progress in these areas, together with system-level integration of HTSE with advanced nuclear and renewable energy sources, is expected to accelerate the deployment of sustainable hydrogen production technologies in the coming decades.

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5

हाइड्रोजन भंडारण अनुप्रयोगों के लिए ठोस-अवस्था पदार्थों की वर्तमान प्रगति और भावी दृष्टिकोण

Current Progress and Future Perspectives of Solid-state Materials for Hydrogen Storage Applications

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सारांश

ठोस-अवस्था हाइड्रोजन भंडारण में धातु हाइड्राइड, उच्च पृष्ठीय क्षेत्रफल वाले मैट्रिक्स तथा रासायनिक/कॉम्प्लेक्स हाइड्राइड जैसे पदार्थों का उपयोग हाइड्रोजन को सुरक्षित रूप से उच्च घनत्व और अपेक्षाकृत कम दाब पर अवशोषित एवं संग्रहीत करने के लिए किया जाता है। यह पारंपरिक हाइड्रोजन भंडारण प्रणालियों से संबंधित आयतन तथा सुरक्षा संबंधी समस्याओं का समाधान करता है, जिससे यह स्थिर विद्युत आपूर्ति, विद्युत ग्रिड के लोड संतुलन तथा शून्य-उत्सर्जन वाहनों के लिए एक उपयुक्त विकल्प बनता है। प्रस्तुत लेख में ठोस-अवस्था हाइड्रोजन भंडारण के लिए विभिन्न संभावित पदार्थों तथा रासायनिकी वर्ग में चल रहे संबंधित अनुसंधान कार्यों पर चर्चा की गई है।

ABSTRACT

Solid-state hydrogen storage uses materials like metal hydrides, high surface area matrix and chemical/complex hydrides to safely bind and store hydrogen at high densities and lower pressures. It resolves the volume and safety issues of conventional storage, making it ideal for stationary power, grid balancing, and zero-emission vehicles. In the present article different candidate materials for solid state hydrogen storage and the on-going research in Chemistry Group are discussed.

KEYWORDS: Hydrogen storage materials, Metal Hydrides



धातु हाइड्राइड के रूप में हाइड्रोजन भंडारण-मिश्रधातु।

Hydrogen Storage in the form of metal hydride

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Introduction

Solid state hydrogen storage materials are solid substances that can absorb, bind, or react with hydrogen to store it safely and efficiently with high densities [1]. They provide a compact, low-pressure alternative to conventional hydrogen storage methods such as compressed hydrogen gas or cryogenic liquid hydrogen, which is critical for making hydrogen fuel viable for vehicular applications and clean energy grids. Storing hydrogen in its pure form presents severe physical challenges. Storage in high pressure cylinder requires extreme pressures (up to 700 bar), which demands heavy, expensive, and potentially hazardous cylindrical tanks. Hydrogen stored in the liquid form requires cryogenic cooling to -253°C , consuming massive amounts of energy just to maintain the temperature. More conveniently, solid state hydrogen storage materials pack hydrogen atoms or molecules closely together inside a solid matrix by chemical or physical interaction, allowing high volumetric density at or near room temperature and ambient pressure. Extensive research is being pursued in the attempt to develop cost effective hydrogen storage materials with high storage capacity, favourable thermodynamics and kinetics for hydrogen charging-discharging and good cyclic stability for both heavy duty vehicle and stationary applications such as heat storage, heat pump, air conditioning of building etc. However, due to practical consideration regarding gravimetric storage capacity at ambient temperature and pressure, the use of solid state hydrogen for vehicular application poses the most demanding challenges for onboard hydrogen storage and delivery. Comparatively lower hydrogen storage capacities can be accepted for stationary applications as weight and volume are not limiting factors in this case.

The hydrogen storage properties of different types of solid state materials have been explored extensively worldwide

and are summarized in Table-1. The various solid state hydrogen storage materials have their own merits and limitation and some of them show very high capacity, fast kinetics, but poor reversibility, again few materials show excellent reversibility suitable condition of operation, but comparatively poor hydrogen uptake. Various factors responsible for this are binding energy, storage mechanism and types of interaction among hydrogen and storage matrix. Depending on that solid state hydrogen storage materials are broadly classified into three categories.

Physical Adsorption on Solid State Materials (Physisorption)

Porous, high-surface-area materials bind hydrogen molecules (H_2) weakly to their surfaces through Van der Waals forces. Key examples are carbon nanotubes (CNTs), graphene oxide, metal-organic frameworks (MOFs), and covalent organic frameworks (COFs) (Fig.1). They are characterised by their fast absorption and desorption cycles, and good cyclic stability, but typically require cryogenic temperatures -196°C to store substantial amounts of hydrogen. Several works have been carried out both theoretically and experimentally in Chemistry Group, BARC, to optimize the interaction energy of hydrogen with the carbon-based materials by modifying low-dimensional nanostructured carbons (such as carbon nanotubes and graphene oxide) to overcome their weak ambient-temperature hydrogen affinity and to maximize storage capacity and stability. Functionalized graphene oxide and heterostructures addresses the poor ambient-condition performance of conventional carbon frameworks by incorporating advanced chemical modifications. Our recent research found that, the use of unconventional highly functionalized graphene oxide (HGO), instead of standard graphene oxide (GO), increases the surface functional group density tremendously, which allows a vastly superior distribution and higher loading of palladium (Pd)



Table-1: Hydrogen storage performance comparison of various solid state hydrogen storage materials.

Sr. No	Material Class	Capacity (wt.%)	Storage mechanism	Kinetics	Operating Temperature	Reversibility	Examples	Technology Maturity	Ref.
1	Carbon based materials	1-7	Physisorption	Excellent	Very low	Excellent	CNTs, graphene	Medium	2
2	Chemical Hydrides	8-20	Covalent bonding	Good	Medium	Poor	NH_3BH_3 , NaBH_4	Medium	3
3	Porous materials	1-10	Physisorption	Excellent	low	Excellent	MOF-5, COF-1	Medium	4
4	HEA Hydrides	1-3.8	Chemisorption	Good	Medium	Good	Ti-Zr-Sc-Cr-V-Ni	Emerging	5
5	Complex Hydrides	5-18	Ionic-Covalent bonding	Moderate	Medium-high	Poor	NaAlH_4 , LiAlH_4	Medium	3
6	Intermetallic Hydrides	1-4.0	Chemisorption	Excellent	Medium	Good	LaNi_5 , Ti-Cr-V	High	13
7	Mg-based Hydrides	5-7.6	Chemisorption	Poor	High	Moderate	MgH_2 , Mg_2NiH_4	High	17



nanoparticles across the sheets, enabling enhanced hydrogen adsorption of 6.62 wt.% with reversibility and excellent retention capacity [6]. Apart from that the heterostructure composed of MXene-graphene oxide combines the high surface area of graphene with the catalytic metallic nature of MXenes creates a synergistic effect that boosts total gas absorption capacity establishing a total capacity of 5.26 wt.% at 173 K [7]. CNT architectures optimisation is carried out by *ex-situ* metal doping, to trigger the “hydrogen spillover” effect—where molecular hydrogen dissociates on a metal catalyst and migrates onto a carbon support. Our research showed that the finely dispersed 3–5 nm size Pd nanoparticles interact directly with the CNT support, enhancing the hydrogen spillover efficiency [8]. Even the synthesis method plays a very important role towards the enhancement of the spillover effect. Comparative evaluations of wet impregnation, polyol methods and reverse micellar route for dispersion of Pd nanoparticle on CNT support showed that the reverse micellar pathway achieves the most stable and uniform dispersion [9]. Apart from the metal doping, in-situ non-metal doping also plays major role towards the hydrogen storage in CNT. Chemical alterations via boron and nitrogen co-doped carbon nanotubes, chemically polarize the carbon lattice, making it more favorable for hydrogen molecules to bind at ambient conditions. Our study showed that the BCNT-based systems can achieve capacities of 2.5 wt.% at 77 K through localized dipoles created by 3.86 at % boron substitution. Structural evolution of porous and turbostratic carbons showed that the structural disorder and geometry of the pure carbons dictate the gas absorption capacity [10] and the chaotic misorientation of carbon layers influence localized hydrogen storage parameters. DFT modeling of carbon-like nanostructures are also considered as a very useful tool for optimisation of the hydrogen storage

properties. Using computational plane-wave pseudopotential methods, the binding mechanism of hydrogen with titanium-decorated silicon carbide (SiC) sheets and (10,0) single-walled SiC nanotubes was established. The DFT calculations demonstrated that titanium decoration distorts the atomic grid of SiC, allowing each Ti metal atom to bind up to four hydrogen molecules with an optimal, reversible average binding energy of 0.37 to 0.65 eV [11].

Metal Hydrides

Certain metals or alloys react chemically with hydrogen, breaking the H_2 molecule apart and storing individual hydrogen atoms within the interstitial spaces of the metal's crystal lattice. Key examples are MgH_2 , $LaNi_5$, TiFe, and body-centered cubic (BCC) alloys. Metallic hydrides are exceptionally safe and possess high volumetric storage capacity at room temperature and ambient pressure. However, they are often heavy and require high temperatures to release the trapped hydrogen. The research on metal hydrides and solid-state storage alloys in Chemistry Group, BARC focuses heavily on engineering multi-component alloy systems to operate under optimal thermodynamic and kinetic windows. The major research approaches targets specific pitfalls of raw metal hydrides like severe thermodynamic stability (requiring excessive release temperatures) and sluggish, multi-stage absorption/desorption kinetics. Among different metal hydride systems, advanced Ti-Cr-V based body-centered cubic (BCC) alloys were found to be highly promising, because they achieved high volumetric storage capacities (~4 wt%) at moderate temperature and pressure (Fig. 2). Modifications of their internal chemical compositions fine-tune their hydrogen storage properties. Zr Substitution for Ti in

$Ti_{0.43}Zr_{0.07}Cr_{0.25}V_{0.25}$ alloy demonstrated that substituting titanium with zirconium drops the hydride desorption temperature by roughly 50 K. This indicated a substantial lowering of the system's overall thermodynamic stability, making hydrogen extraction significantly easier [12]. The inclusion of secondary Laves phases alongside the main BCC matrix also altered hydrogen storage properties. The phase configuration acted as a kinetic highway, allowing fast hydrogen capture without requiring prolonged initial activation cycles. Transition metal doping in $Ti_{2x}CrVM_x$ ($x = Fe, Co, Ni$) alloys showed that the addition of elements like nickel or iron weakened localized metal-hydrogen binding, preventing the framework from locking up the hydrogen permanently [13]. The substitution behavior of iron, vanadium, and zirconium within $LaNi_5$ -type classical alloys showed that the vanadium-substituted formulations $LaNi_4V_{0.5}Fe_{0.5}$ created flat, highly reproducible pressure-composition-temperature (PCT) isotherm plateaus near 1 bar at room temperature, required for room-temperature operational capability. This makes it perfectly balanced for commercial distribution systems, whereas zirconium substitution results in uneven, sloped operational pressures [14]. While magnesium hydrides, MgH_2 , have high storage capabilities by weight (7.6 wt.%), they typically require operational temperatures exceeding 300°C. Density Functional Theory (DFT) modeling and experimental surface studies showed that the transition metal catalysis like Ti, V, and Ni modulate the dissociation and diffusion kinetics of

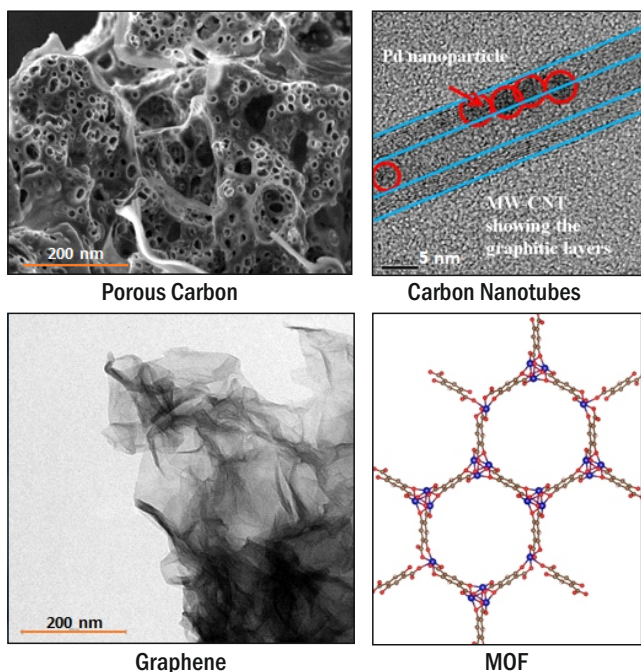
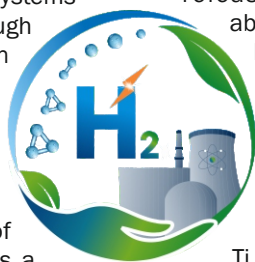


Fig.1: Different classes of materials for hydrogen storage by physisorption.

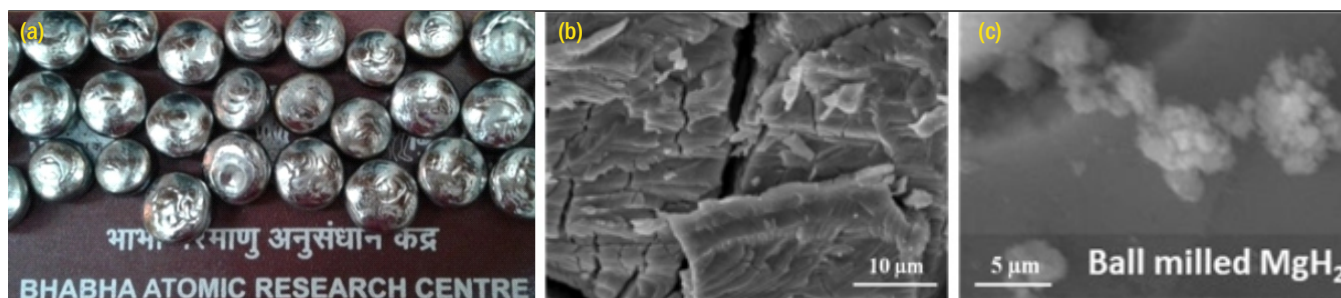


Fig.2: Hydrogen Storage in the form of metal hydride (a) Alloy (b) Scanning Electron Microscopy of pulverised metal hydride (c) Ball milled magnesium hydride.

hydrogen on Mg(0001) surface [15]. Theoretical calculation proved that placing transition metals on the surface or subsurface layers dramatically lowers the energy barriers required to split the H_2 molecule apart. Modeled small Ti-doped magnesium clusters $TiMg_{54}$ and $TiMg_8$ showed that structural scaling down to the nanoscale alters the electron density, which forces immediate molecular dissociation and atomic diffusion into the internal storage sites at much lower thermal inputs [16]. Detailed hydriding mechanism and kinetics analysis study in the engineer scaled storage reactors, maps out exactly how hydrogen travels into bulk metals. Using standard kinetic fitting equations on experimental data showed that hydrogen atoms after dissociation on the surface travel inside the engineered nano-magnesium and are bounded first by random atomic nucleation, followed by 1D and 3D diffusion through the formation of hydride surface layer [17].

Chemical and Complex Hydrides

Chemical and complex hydrides represent a major class of solid-state hydrogen storage materials capable of binding hydrogen via strong covalent or ionic chemical bonds. Unlike physical adsorption materials, that require cryogenic temperatures, these hydrides achieve exceptionally high volumetric and gravimetric hydrogen densities at or near ambient conditions. Major classes of complex hydrides feature a central metal or non-metal atom covalently bound to hydrogen, forming a complex anion paired with a light metal cation: Sodium borohydride ($NaBH_4$) and Lithium borohydride ($LiBH_4$) boast immense theoretical hydrogen storage capacities. Hydrogen release from air-stable $NaBH_4$ is typically triggered via catalytic hydrolysis. Sodium alanate ($NaAlH_4$) is the most widely studied complex hydride. It releases hydrogen in a multi-step thermal decomposition path. Doping it with titanium (Ti) catalysts makes the reaction reversible under practical conditions. Systems like Lithium amide ($LiNH_2$) store up to (6.5 wt.%) hydrogen, when reacted with lithium hydride (LiH). They function via a reversible amide-to-imide phase transformation pathway. Chemical hydrides store hydrogen within molecular compounds and release it through a breakdown of their primary chemical structure. Ammonia Borane (NH_3BH_3 , AB) contains both hydridic (B-H) and protonic (N-H) hydrogens, creating a high-density molecular crystal (19.6 wt.% hydrogen). It releases hydrogen at low temperatures via catalytic hydrolysis or at high temperature by stepped thermal decomposition.



The research on ammonia borane (NH_3BH_3 , AB) in Chemistry Group, BARC centers around the development of highly efficient, recyclable catalysts (Fig.3) to unlock its massive theoretical hydrogen storage capacity (19.6 wt.%). Ammonia borane suffers from sluggish hydrogen release at room temperature and generates volatile impurities like ammonia (NH_3) gas; as a result the research work mainly focuses on catalytic hydrolysis to ensure safe, room-temperature green hydrogen production. Designing specialized support matrices to highly disperse metal nanoparticles, lowers the activation energy (E_a) required for snapping the molecular bonds of AB. A green synthesis method using electron beam irradiation was developed, to decorate palladium nanoparticles (<10 nm) on a graphitic carbon nitride matrix demonstrating that the catalyst slashed the hydrolysis activation energy to an impressively low ($27.36 \text{ kJ mol}^{-1}$) [18]. Biomass-derived cost-effective, porous carbon supported palladium nanoparticles, yielded a 3.4-fold reduction in activation energy compared to uncatalyzed AB hydrolysis [19]. Engineered magnetically separable copper-iron oxide polymer beads ($Cu@Fe_3O_4:PES$) provided a scalable, non-noble metal alternative for rapid hydrogen evolution from AB [20]. A major challenge with ammonia borane hydrolysis is the co-release of trace ammonia gas, which can poison fuel cell membranes. Recent work on pore-engineered, non-noble metal ZIF-67 (Zeolitic Imidazole Frameworks) acted as a dual-function matrix, which catalyzed the hydrogen generation reaction showing remarkably low activation energy of $15.63 \text{ kJ mol}^{-1}$, while chemically trapping and mitigating released ammonia [21]. Pd-dispersed MOFs were also developed, that enable ammonia-free hydrogen generation from both ammonia borane and sodium borohydride in aqueous solutions [22]. To completely avoid reliance on metal based catalysts, use of macrocyclic “nanocavitands” was established to structurally manipulate the AB molecule, demonstrating a metal-free supramolecular strategy, where cucurbit[5/8]uril nanocavitands encapsulate ammonia borane. This lowered the hydrolysis activation energy from $103.8 \text{ kJ mol}^{-1}$ down to 27.5 kJ mol^{-1} , matching the performance of expensive platinum and palladium metal nanoparticles—while significantly suppressing unwanted volatile ammonia release [23]. Utilizing time-dependent FT-IR and mass spectrometry study coupled with Kinetic Isotope Effects (KIE) proved that the evolved hydrogen gas originating from a synchronized splitting of both

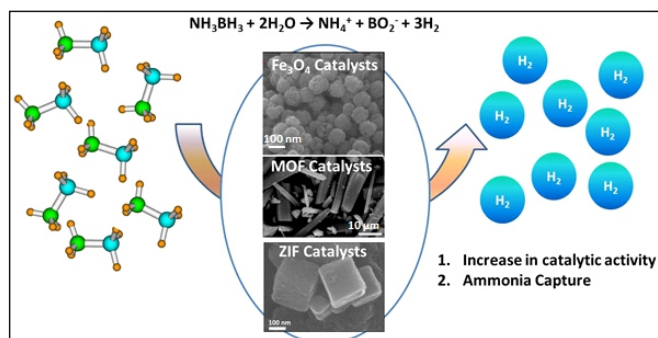


Fig.3: Room temperature hydrogen release from ammonia borane in presence of different catalysts.

the internal (B–H) bonds of ammonia borane and the (O–H) bonds of the surrounding water solvent.

Way forwards

Recent research on hydrogen storage is shifting from heavy, rare earth metal hydrides to lightweight alternatives such as vanadium-based, magnesium-based alloys and light element based complex frameworks. These allow for higher hydrogen storage capacities and faster absorption/desorption rates at near-ambient temperatures. To solve the challenge of transporting compressed or cryogenic hydrogen, developers are testing solid-state hydrogen storage technologies (like hydrogen-rich powders) that can be easily transported at low pressures and later processed to release clean fuel. To become viable for mainstream automotive and stationary applications, storage materials are required to hit specific targets, including a cost-effective production benchmark, moderate operating temperatures, and a maximum hydrogen weight percentage. While long-term adoption aims to fuel zero-emission vehicles, the immediate way forward focuses on stationary energy storage, remote off-grid community power, and microgrids where the safety and compact footprint of solid-state hydrogen storage systems outweigh traditional high-pressure tanks.

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6

2D नैनो-पदार्थों में प्रतिवर्ती हाइड्रोजन भंडारण का अन्वेषण: घनत्व डोपिंग एवं तनाव के माध्यम से वृद्धि

Exploring Reversible Hydrogen Storage in 2D Nanomaterials: Enhancement Through Doping and Strain

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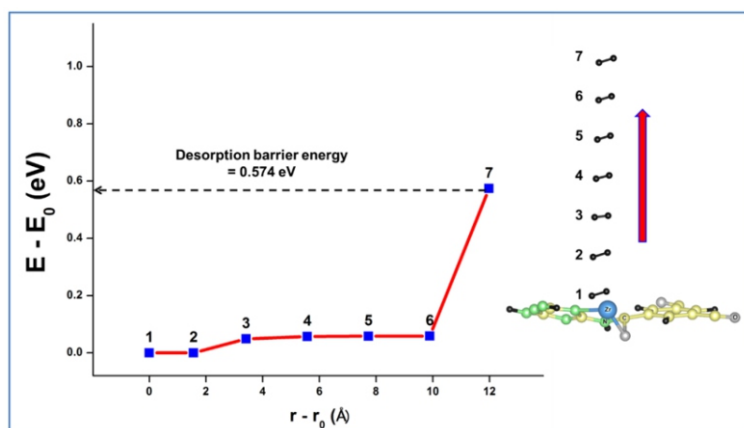
सारांश

हाइड्रोजन भंडारण एक स्वच्छ ऊर्जा वाहक के रूप में हाइड्रोजन के व्यावहारिक उपयोग और व्यापक रूप से अपनाए जाने हेतु एक महत्वपूर्ण सहायक है, जो अक्षय ऊर्जा एकीकरण को सुविधाजनक बनाता है और विभिन्न क्षेत्रों के विकास का समर्थन करता है। विभिन्न 2D नैनो-पदार्थों ने अपने उच्च सतह क्षेत्र, उच्च चालकता एवं उच्च यांत्रिक शक्ति के कारण ऊर्जा भंडारण उपकरणों के रूप में अत्यधिक ध्यान आकर्षित किया है। हालांकि H₂ भंडारण के लिए कार्बन आधारित 2D पदार्थ का पता लगाया गया है, लेकिन यह कमरे के तापमान पर H₂ को नियंत्रित नहीं कर सकता है क्योंकि अंतःक्रिया बहुत कमजोर है। यह देखा गया है कि 2D पॉलीआरामिड (2डीपीए), संक्रमण धातु (टीएम) परमाणुओं की एकल इकाई सेल को सजाकर, -0.399 और -0.480 eV की औसत बाध्यकारी ऊर्जा के साथ H₂ के 6.422 और 6.792 wt% तक के हाइड्रोजन भंडारण को क्रमशः 2DPA+Ti और 2DPA+Zr के लिए प्राप्त किया गया, जो हाइड्रोजन भंडारण उपकरणों के लिए डीओई की आवश्यकता को पूरा करता है। अध्ययन एक कुशल एवं प्रतिवर्ती हाइड्रोजन भंडारण पदार्थ के रूप में तनावग्रस्त 2D होले ग्रेफाइन की क्षमता पर भी प्रकाश डालता है।

ABSTRACT

Hydrogen storage is a crucial enabler for the practical use and widespread adoption of hydrogen as a clean energy carrier, facilitating renewable energy integration and supporting the decarbonization of various sectors. Various 2D nanomaterials have drawn immense attention as energy storage devices due to their high surface area, high conductivity and high mechanical strength. Although carbon based 2D materials have been explored for H₂ storage, it can't hold H₂ at room temperature because interaction is very weak. It has been shown that by decorating a single unit cell of 2D polyaramid(2DPA) by transition metal (TM) atoms, hydrogen storage of up to 6.422 and 6.792 wt% of H₂ with average adsorption energies of -0.399 and -0.480 eV have been obtained for 2DPA+Ti and 2DPA+Zr, respectively, satisfying DoE's requirement for hydrogen storage devices. The study also highlights the potential of strained 2D holey graphyne as an efficient and reversible hydrogen storage material.

KEYWORDS: Hydrogen storage, 2D materials, Density Functional Theory, Green economy, Strain Engineering, Kubas interactions



CI-NEB विधि का उपयोग से संगणित
2DPA+Zr+H₂ प्रणाली से हाइड्रोजन के
अवशोषण हेतु ऊर्जा बाधा।

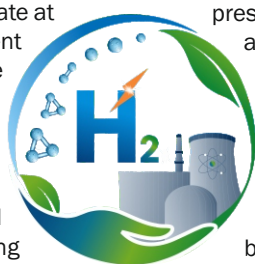
Energy barrier for desorption
of hydrogen from 2DPA+Zr+H₂
system computed using CI-NEB
Method

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Introduction

One of the major societal concerns that need to be addressed is that of the energy crisis, as the usage of fossil fuels gives rise to myriad problems. The dependence of humans on fossil fuels for energy, especially for transportation, poses immense threat to the future of human life. Not only do fossil fuels release greenhouse gases that contribute to climate change, but even the supply of fossil fuels is limited and we may soon run out of it. Thus, there is dire need to find an alternative to fossil fuels, and one that does not release harmful emissions or by-products is much desirable. Fuel cells have been touted as possible replacements for the internal combustion engine for mobile energy harnessing, and were made very popular by the Apollo Space mission when the alkaline fuel cells designed by Francis Bacon were used as an onboard energy producer, as well as water provider, given that a hydrogen-oxygen fuel cell produces water as a by-product [1]. For light vehicles however, the storage of hydrogen on the vehicle presents a major challenge. Hydrogen storage in compressed gaseous form requires large-volume, high-pressure cylinders [2], whereas storage in liquid form involves energy-intensive cryogenic liquefaction and the use of reinforced storage vessels. The storage and transportation of hydrogen in its liquid or gaseous form may be too cumbersome for an ordinary light vehicle. Instead, the adsorption of hydrogen on a solid substrate at a re-fueling site, and its desorption during requirement can be an effective solution for this issue, much like how a fuel tank operates today. Hydrogen has the highest known energy density among fuels with an achievable energy conversion efficiency of up to 65% in a stationary fuel cell-based power plant, compared to the 33–35% achieved for a conventional combustion-based thermal power plant [3]. Using hydrogen fuels emits almost no carbon and greenhouse gases, resulting in a far lower carbon footprint than that observed in conventional fuels & decreased air pollution levels.



The U.S. Department of Energy (DOE) [4] has established specific performance targets that solid-state materials must meet for practical, reversible hydrogen storage. To be viable for light-duty vehicles, current targets specify a hydrogen-substrate binding energy of -0.2 to -0.7 eV and a minimum gravimetric storage capacity of 6.5 wt%. Efficient solid-state hydrogen storage requires a balanced binding energy between physisorption and chemisorption. Developing such a material is challenging because it must simultaneously be lightweight, economical, high-capacity, and stable over thousands of cycles, while allowing effortless hydrogen release via minor temperature or pressure adjustments.

This article describes the conventional materials used for hydrogen storage, their merit and demerit. It also highlights computational design of new generation light element based 2D materials for efficient and compact storage of molecular hydrogen. It emphasizes various interaction mechanism of H₂ molecules on different materials, e.g. on pristine carbon based 2D material, transition metal doped 2D materials, strained 2D materials, non-metal substituted 2D materials etc. It also describes how to enhance hydrogen adsorption on light elements based 2D materials due to strain, doping of transition metals and substitution of non-metals.

Conventional materials used for hydrogen storage

Metal hydrides are well-explored substrates for solid-state hydrogen storage, where hydrogen atoms are incorporated into the crystalline structure of metals or metal alloys. For example, complex metal hydrides such as alanates (e.g., NaAlH₄) and borohydrides (e.g., LiBH₄) have been extensively studied [5,6]. Also, La-Ni hydride (LaNi₅H₆) has been explored as high capacity media for hydrogen storage. These materials can store significant amounts of hydrogen by weight but often require high temperatures for hydrogen release, limiting their practical use in certain applications. Another class of materials for solid state hydrogen storage includes porous materials such as metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) [7]. These materials feature large surface areas and well-defined nanoporous structures, which facilitate hydrogen adsorption through weak van der Waals (vdW) forces. MOFs like MIL-101 [8] and COFs such as COF-105 and COF-108 have shown promise due to their tuneable properties and high hydrogen storage capacities under specific conditions [9]. However, practical challenges such as slow kinetics and material degradation must be addressed for widespread commercial use. Zeolites, known for their cage and channel structures can adsorb non-polar gases through physisorption [10]. The Na-Y zeolite can provide 1.81 wt% hydrogen uptake at 77 K and pressures of 1.5 Mpa [11]; whereas, Na-X gave 2.55 wt% at 77 K and pressures of 40 bar [12]. While zeolites show rapid hydrogen adsorption-desorption, the adsorption mechanism is primarily via physisorption. Owing to the poor adsorption strength, hydrogen storage in zeolites necessitates low operating temperatures (preferably, cryogenic conditions) and high hydrogen pressures. These may be achievable for stationary storage purposes but become cumbersome for onboard hydrogen storage in transport applications.

2D Nano-materials: Next generation Hydrogen Storage Devices

2D materials are a class of crystalline solids with atomic scale thickness and lateral dimensions extending up to the nm or micron scale. Since the ground breaking discovery of graphene, extensive research has led to the identification and development of a wide variety of 2D materials, which can be classified based on their elemental composition, bonding nature, and structural

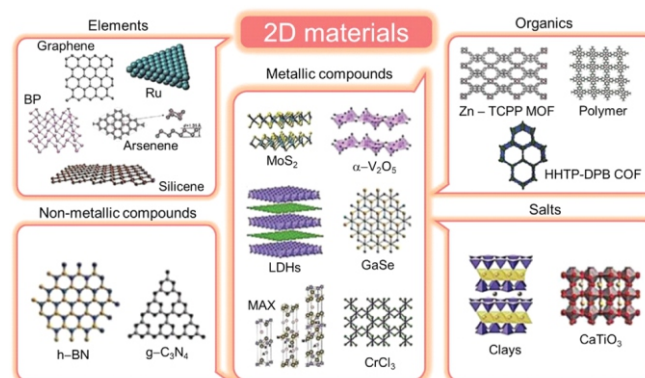


Fig.1: The atomic structures of different types of newly discovered two-dimensional material categories are schematically shown here [18].

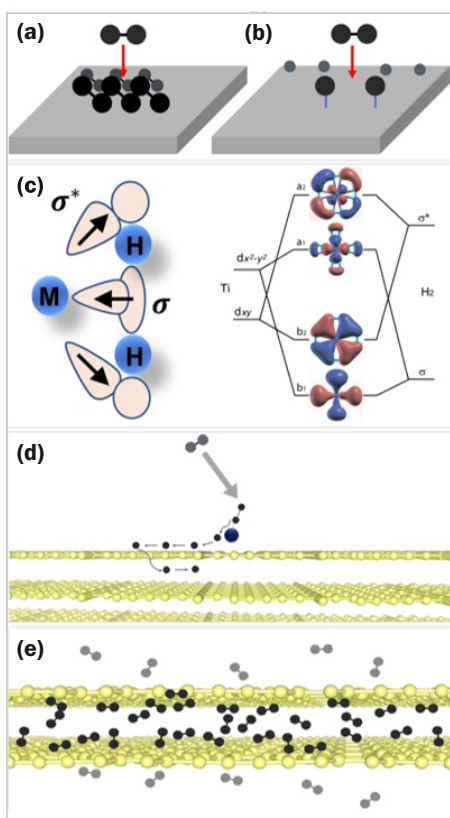


Fig.2: Mechanisms of solid-state hydrogen storage; (a) physisorption involving molecular hydrogen attracted to the substrate surface via van der Waals forces; (b) chemisorption involving dissociative adsorption of hydrogen; (c) Kubas interactions showing, in the left panel,† back donation of charge from σ^* orbitals of H_2 to the vacant d orbitals of the transition metal, and in the right panel, molecular orbital diagram showing hybridization between Ti and H_2 molecular orbitals;‡ (d) spillover mechanism of H_2 dissociating on a catalyst-embedded nanomaterial; and (e) nanopump effect in few-layer 2D materials. The yellow and black spheres denote C and H atoms, respectively; reproduced from Solid State Commun. 147, 419–422, 2008 [22].

properties. The first category includes elemental 2D materials, composed of a single type of atom arranged in a 2D lattice such as graphene (C), phosphorene (P), silicene (Si), germanene (Ge), and borophene (B) etc. These materials exhibit exceptional properties like high conductivity, flexibility, and mechanical strength. Another major category is transition metal dichalcogenides (TMDs), typically represented by the formula MX_2 , where M is a transition metal (e.g., Mo, W, Nb, Ta, Ti etc.) and X is a chalcogen (e.g., S, Se, Te) [13, 14]. TMDs exhibit semiconducting, metallic or superconducting behavior and are widely used in electronics, optoelectronics, and catalysis. Hexagonal boron nitride (h-BN), often called “white graphene,” is an insulating 2D material with excellent thermal and chemical stability [15]. In recent years, attention has also been drawn to Mxenes [16, 17], a family of transition metal carbides, nitrides, or carbonitrides with outstanding electrical conductivity and surface functionality, making them promising for energy storage, sensing, and catalytic applications. A similar but newer class is MBenes, which is a family of 2D transition metal borides derived from MAB phases, possessing high mechanical strength and favorable electronic properties for catalysis and sensor applications.

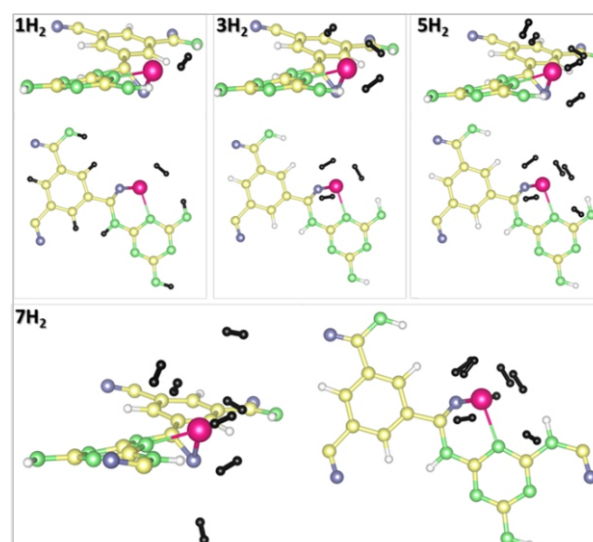


Fig.3: Structural plots in the top and side views for $2DPA+Ti+nH_2$ where $n = 1, 3, 5$, and 7 . Yellow, green, gray, white, and pink spheres represent the C, N, O, H, and Ti atoms of $2DPA + Ti$, respectively. Black spheres represent the adsorbed hydrogen molecules [29].

In last few years several graphene based 2D materials have been synthesized by modifying the elemental graphene structures with hetero-atom, different hybridized carbon atoms or incorporating different functional groups which includes graphyne, holey-graphyne, BeN_4 , biphenylene, C_6N_7 , C_5N , 2D Polyaramid etc. Fig.1 illustrates these different types of two-dimensional materials [18].

Interaction mechanism of H_2 with pristine and functionalized 2D materials

Pristine carbon nanomaterials are typically poor hydrogen adsorbers. Their electronic structure does not provide strong interactions with hydrogen molecules, leading to weak adsorption solely due to vdW forces. Modifying these materials, by introducing defects, functional groups, or doping with other elements, can alter their electronic properties and create more active sites, enhancing their hydrogen adsorption capacity. The binding of hydrogen via physisorption or chemisorption in solid substrate has been considered as a traditional mechanism [19]. As per the International Union of Pure and Applied Chemistry (IUPAC), physisorption is predominantly due to the vdW forces that arise between the adsorbate and adsorbent [18]. The electronic structure of the participating species remains unchanged in physisorption owing to the weak nature of vdW forces ($< 10 \text{ kJ mol}^{-1}$) [20]. The energy barrier for physisorption is low and typically, hydrogen physisorption has rapid adsorption/desorption kinetics. Additionally, the hydrogen storage capacity in such materials is also far too low to satisfy the DOE criteria. In contrast, chemisorption involves the introduction of atomic hydrogen into the crystal lattice of the substrate which may diffuse and occupy the interstitial sites. Consequently, the enthalpy of hydrogenation is high for hydrides, and necessitate high desorption temperatures to overcome the high energy barriers. The specific requirements for onboard reversible hydrogen storage in FCVs, and particularly in light-duty FCVs, call for a hydrogen binding mechanism that provides adsorption

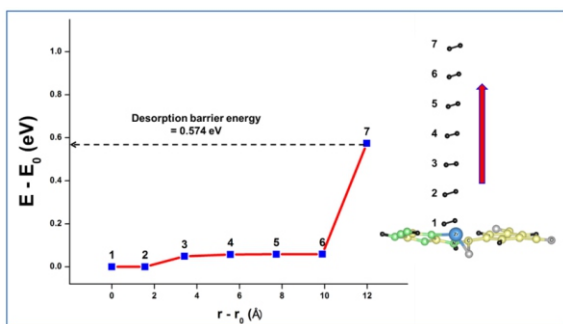


Fig.4: Energy barrier for the desorption of hydrogen from 2DPA+Zr+H₂ system computed using the climbing nudged elastic band method [29].

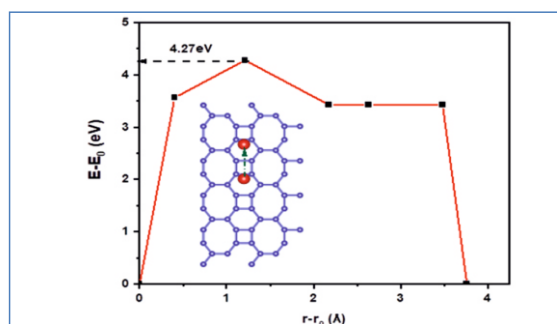


Fig.6: Diffusion Energy barrier of Bph + Nb system computed using CL-NEB Method [31].

energies intermediate to that of physisorption and chemisorption. The weak van der Waals interactions can be enhanced by introducing electric field through strain, defects or non-metal substitution. Another mechanism is Kubas interactions between transition metals and hydrogen. Kubas binding, elucidated by Gregory Kubas, describes a distinctive interaction mechanism between hydrogen molecules and TM complexes (Fig.2) [21]. In this interaction, hydrogen molecules approach the TM centre where they donate electron density from their σ -orbital the bonding orbital containing electron density to an empty d orbital or hybrid orbital of the TM. Concurrently, the TM complex back-donates electron density from its filled d orbitals or hybrid orbitals into the anti-bonding orbitals of the hydrogen molecule. This exchange of electron density creates a bond that is intermediate between chemisorption, involving strong chemical bonds, and physisorption, which relies on weaker vdW forces. The Kubas binding mechanism is notable for its ability to enhance hydrogen adsorption capacities of materials containing TMs, thereby offering potential applications in hydrogen storage technologies. The different interaction mechanisms are depicted in Fig.2 [22].

Computational Details

Theoretical simulations can provide a clear picture regarding adsorption configuration, adsorption energy, charge transfer and orbital interactions which are difficult to get in experiments. In this respect, Density Functional Theory is a rapid method in computational chemistry for computing the ground

state energy, electronic, magnetic, etc., properties of materials. In place of solving the Schrodinger equation for the wave function to obtain the energy, DFT uses the probability density of electrons, or electron density which involves lesser variables and is therefore rapid while being quite accurate.

The DFT calculations in this work have been performed using the projector-augmented wave formalism implemented in the Vienna ab initio Simulation Package (VASP) [23, 24]. Conjugate gradient methods were used for structural relaxation and the energy and interatomic force threshold for convergence was set at 10^{-5} eV and 0.01 eV/Å.

We have accounted for dispersion corrections by implementing Grimme's DFT-D3 scheme in all the calculations [26]. To find the structural stability at higher temperature, we have used Ab-initio Molecular Dynamics simulations (AIMD). The AIMD simulations utilized in these studies involved two stages. In the first stage, the system was heated from 0 K to 300 K (or higher) in an NVE ensemble in one-femtosecond timesteps for a time-period of around 5-10 picoseconds. Thereafter, the system was further equilibrated for another 5-10 picoseconds in an NVT ensemble with the temperature maintained at 300 K (or higher) using the Nose-Hoover thermostat. To find the dynamic stability, Phonon dispersion calculations were performed with increased convergence threshold values of energy cutoff (10^{-8} eV) and interatomic forces (10^{-3} eV/Å) and the Phonopy code was utilized to plot the phonon spectrum [27]. The climbing nudged elastic band (CI-NEB) method was utilized to analyze hydrogen desorption behavior.

Mechanism to Enhance Hydrogen Adsorption

For pristine light elements based 2D materials, interactions with H₂ is very weak, giving an adsorption energy around -0.10 eV/H₂, lower than DoE requirement. This adsorption is due to weak Van Der Waal's interactions and the system can't hold H₂ molecules at ambient condition. Different strategies have been adopted to increase the adsorption energy of H₂ so that system can store H₂ at ambient condition. In this article, we will discuss some of our recent work employing following strategies:

- Transition metal doping
- Applying external strain
- Non-metal substitution

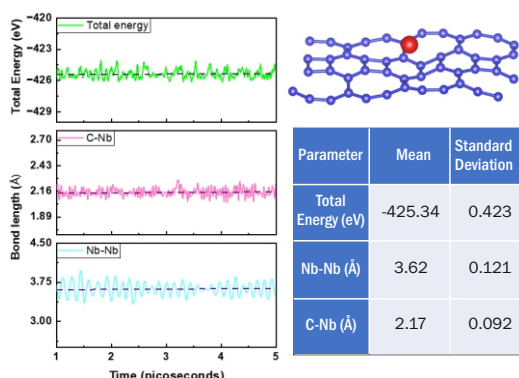


Fig.5: Time variation of Energy (top panel), and Bond lengths (bottom panels) of C-Nb and Nb-Nb bond are plotted with time (picoseconds) and distance (Å). The mean and standard deviations of the same are shown in the table [31].



Table 1: Summary of the hydrogen storage performance of 2DPA+Ti and 2DPA+Zr [29].

System	Binding energy/H ₂ (eV) with DFT-D2 corrections	
	2DPA+Ti	2DPA+Zr
2DPA+TM	-2.712	-4.122
2DPA+TM+1H ₂	-0.513	-0.544
2DPA+TM+3H ₂	-0.338	-0.509
2DPA+TM+5H ₂	-0.419	-0.555
2DPA+TM+5H ₂	-0.279	-0.429
2DPA+TM+9H ₂	NA	-0.365
Average binding energy/H ₂ (eV/H ₂)	-0.399	-0.480
Average desorption temperature (K) at 5bar	328.76	395.08

Enhancing hydrogen adsorption through Transition metal Doping

We have explored few novel 2D material to enhance their hydrogen adsorption capability by doping early transition metals(TM) with minimum unpaired electrons in the outermost shell as those TMs are good hydrogen absorber.

Titanium and zirconium decorated 2DPA nanosheet

2D polyaramid (2DPA) [28] is a porous and polymeric material which has been synthesized recently. We have studied the hydrogen storage capability of Titanium and zirconium decorated 2DPA nano sheet. By decorating a single unit cell of 2DPA with two transition metal (TM) atoms, hydrogen storage of up to 6.422 and 6.792 wt% of H₂ with average binding energies of -0.399 and -0.480 eV is predicted for 2DPA+Ti and 2DPA+Zr, respectively [29]. The binding of Ti and Zr with 2DPA is accompanied by a flow of charge (-1.474 e for Ti and -1.696 e for Zr) from the TM towards the 2DPA sheet. Table.1 represent a summary of adsorption energy for hydrogen on Ti and Zr doped 2DPA. Further, the interaction between H₂ and TM may proceed via Kubas interaction between the d orbital of the TM in 2DPA+TM and molecular orbitals of H₂, with a net flow of charge from the TM towards H₂ (-0.218 e for Ti and -0.391 e for Zr). The adsorption configurations of various H₂ molecules on 2DPA+Ti is displayed in Fig.3. The desorption of H₂ bound to 2DPA+Zr is endothermic (~0.57 eV) and close in magnitude to the binding energy of the first H₂ (~-0.544 eV) as displayed in Fig.4 where desorption energy barrier of first adsorbed H₂ has been computed using sophisticated CI-NEB method. The 2DPA+TM systems show structural and dynamic stability at high temperatures as evident from ab initio molecular dynamics simulations and phonon spectra. The movement of TM atoms across the 2DPA sheet to form clusters may be hindered by the considerable barrier energy (~4.9 eV for Ti). Through these systematic density functional theory simulations, we predict that Ti- and Zr-decorated 2DPA are high-performance hydrogen storage materials and can be explored by experimentalists.

Niobium decorated 2D Biphenylene nano-sheet

Biphenylene is a two-dimensional non-benzenoid carbon allotrope formed from a series of square, hexagonal and octagonal rings of sp² hybridized carbon atoms [30]. We have explored the hydrogen storage capability of 2D Biphenylene by decorating it with Niobium. Niobium atom gets bonded above the

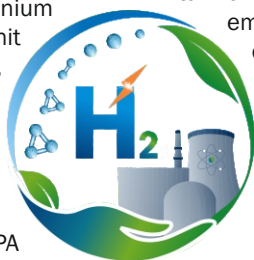
bond between the octagonal and hexagonal ring with binding energy of -3.42 eV due to charge transfer from Nb d orbital to C 2p orbital. If Nb is decorated at all stable configurations, in a unitcell of biphenylene on both sides, the system will have a total of 8 Nb atoms and 40 H₂ molecules providing hydrogen uptake of gravimetric 5.76 wt% with average adsorption energy of 0.61 eV/H₂ [31].

To serve as a viable option in hydrogen storage applications, the materials should be thermally stable at higher temperatures. To analyze the thermal stability of the material, a two-step computational technique called ab initio Molecular Dynamics simulations were performed. Initially, the system was heated from 0 to 300 K over 10ps using an NVE ensemble with a 1fs time step. Subsequently, the material was equilibrated at 300K for another 5ps within an NVT ensemble employing a Nose Hoover thermostat to maintain constant temperature. The time evolution of energy as well as bond lengths are plotted in Fig.5. The negligible fluctuations in bond length and energy ensures the thermal stability of the system at room temperature.

Furthermore, the tendency of transition metals to form clusters, due to their high cohesive energy, might become a setback for their utilization in hydrogen storage application. In the hope of overcoming that, the energy required for the Nb atom to move across two equivalent positions was computed by employing the CI-NEB method. Initially the system was optimized at two equivalent positions and five images of the Nb atom at intermediate positions were generated. The maximum energy barrier, Nb atom must cross to move in the mono layer was found to be 4.27 eV (Fig.6). The high energy barrier reduces the chances of clustering making the system stable for onboard hydrogen storage.

Vanadium attached 2D Aza-triphenylene

Recently, Hao Yang et al. and Kai Niu et al. successfully synthesized a novel two-dimensional (2D) material Aza-triphenylene (Aza-COF) which represents a unique carbon-based covalent organic framework and an advanced carbon allotrope with promising structural and electronic properties [32,33]. Our DFT simulations demonstrate that vanadium-decorated Aza-triphenylene-based covalent organic frameworks (Aza-COF) are promising candidates for onboard, reversible hydrogen storage in light-duty fuel cell vehicles (FCVs). The optimal binding configuration involves vanadium atoms positioned between two nitrogen atoms at the framework edges, enabling stable adsorption of up to seven H₂ molecules per vanadium atom with an average binding energy of -0.46 eV [34], which meets the U.S. Department of Energy (DOE) requirements for hydrogen storage. The system achieves a gravimetric hydrogen uptake of 6.67wt%, approaching DOE targets, while a high diffusion barrier (~6.06 eV) prevents vanadium clustering, ensuring uniform dispersion across the COF surface. To gain deeper insights into the weak intermolecular interactions governing hydrogen adsorption and release in V-decorated Aza-COFs, a Non-Covalent Interaction (NCI) analysis was conducted [35]. As the H₂ molecules are added, the increase in green peaks in the scatter plot and iso-surface indicates dominance of weak Van der Waals interactions as shown in Fig. 7.





Titanium doped 2D - Ψ Graphene

Another advanced 2-D allotrope of carbon, called Ψ - Graphene has been theoretically predicted. It is metallic in nature and comprises of hexagonal, pentagonal and heptagonal rings of carbon [36]. Ψ - Graphene crystallizes with P_{2mg} plane symmetry and contains 12 C atoms in the unit cell having lattice constants as $a=6.70\text{\AA}$ and $b=4.84\text{\AA}$. It is known that the unique arrangement and metallic nature of Ψ - Graphene makes it thermodynamically and mechanically more stable compared to other 2-D allotropes of carbon. We presented the hydrogen adsorption of Ti decorated Ψ - Graphene (advanced 2D allotrope of carbon) using Density Functional Theory simulations [37]. Ti atom is attached strongly on Ψ - Graphene with adsorption energy of -3.39 eV due to transfer of electron from Ti 3d orbital to C 2p orbital. Titanium atom can be loaded on both side of Ψ - Graphene sheet with each Ti adsorbing maximum of 9 H_2 molecules providing gravimetric H_2 uptake of 13.14 wt%, quite higher than the prescription of 6.5 wt % by DoE's. The average adsorption energy of -0.344 eV per H_2 and an average desorption temperature TD of 438.3K provide favorable



thermodynamics for reversible hydrogen storage in fuel cell systems. The adsorption energy of H_2 is in between physisorption and chemisorptions due to Kubas interactions where H 1s orbital receives charge from metal. The interaction of Ti on Ψ - Graphene have been presented by electronic density of states analysis, charge transfer and plot for spatial distribution of charge as displayed in Fig.8. There is orbital interaction between Ti 3d and C 2p of Ψ - Graphene involving transfer of charge whereas bonding of hydrogen molecules is through Kubas type of interactions involving charge donation from σ orbitals of hydrogen molecules to the vacant 3d orbital of Ti and the subsequent back donation to σ^* orbital of hydrogen from filled 3d orbital of Ti. The system (Ψ - Graphene + Ti) was found to be stable at higher temperature by Molecular Dynamics calculations and diffusion energy barrier of 1.6 eV for Ti atom can prevent metal-metal clustering.

Strain Engineering

There are some serious limitations to the mass production of TM-decorated 2D nanomaterials, which hinder their widespread use as next-generation hydrogen-storage materials.

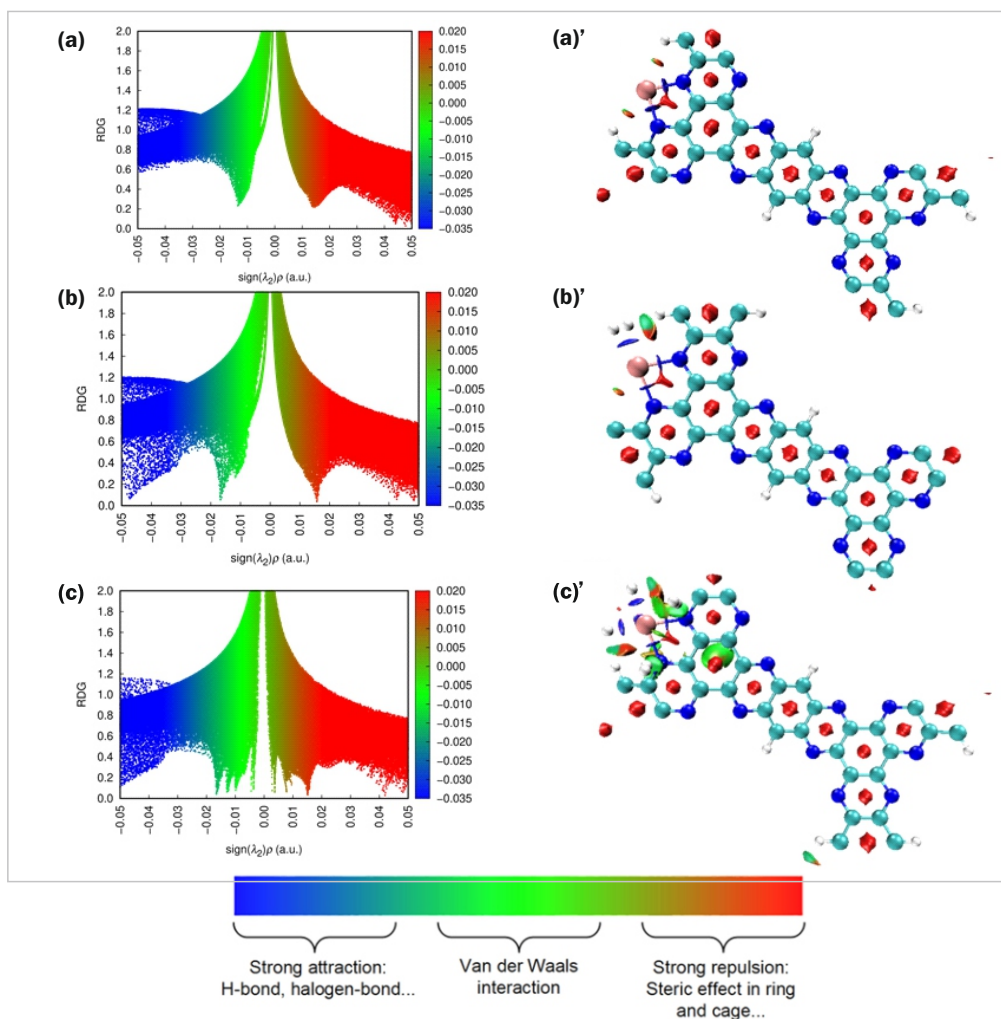


Fig.7: Reduced density gradient (RDG) iso-surfaces and corresponding scatter plots of RDG vs $\text{sign}(\lambda_2)\rho$ for (a,a') Aza-COF+V (b,b') Aza-COF+V+1 H_2 , and (c,c') Aza-COF+V+7 H_2 , respectively [34].

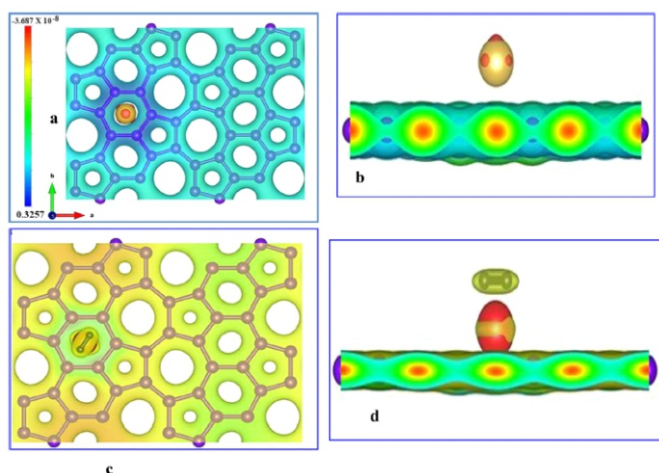


Fig.8: Electron Density plot for electron density difference between Ti-doped ψ -graphene and pristine ψ -graphene for isovalue of 0.106e; (a) top view; (b) side view; electron density plot for electron density difference between $H_2 + Ti + \psi$ -graphene and Ti doped ψ -graphene for isovalue of 0.074e; (c) top view; (d) side view. Charge loss region is indicated by red color and electron gain region by green color (less gain) and blue color (more gain) [37].

Firstly, the synthesis protocol of TM-decorated 2D nanomaterials must be designed to prevent TM aggregation into clusters. Ensuring a uniform distribution of TMs across the nanomaterial substrate is made complex owing to the high cohesive energies of TMs, particularly early TMs, driving them towards cluster formation. In addition, TMs are susceptible to oxidation due to their unique electronic structure characterized by partially filled d orbitals, which allow for multiple oxidation states to occur. Thus, their electronic configuration drives TMs to lose electrons and become cationic, driving them towards forming strong metal-oxygen bonds. These TM oxides are typically stable, making the oxidation process thermodynamically favourable. Furthermore, TMs loaded on nanomaterials exhibit a high specific surface area, increasing their reactivity and propensity for oxidation. Another significant impact of TM loading in nanostructures is the structural integrity of the host material.

Thus, alternative strategies that alter the electronic structure to enhance the substrate's reactivity and conductivity are desirable for designing efficient hydrogen-storage materials. Some of these strategies are outlined here.

Strain engineering involves applying strain in the substrate

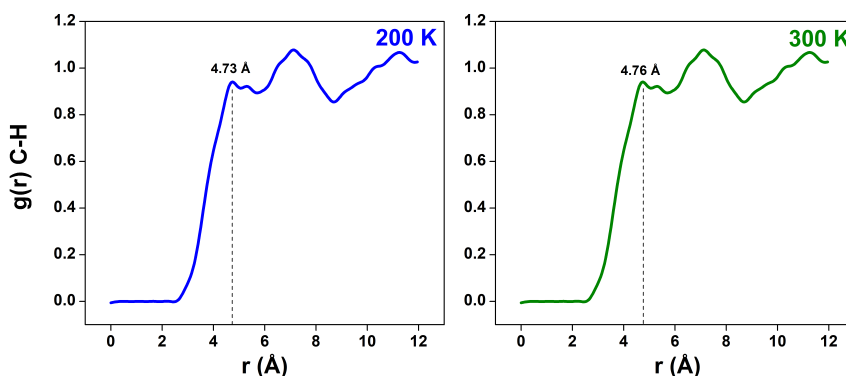


Fig.9: Radial distribution function $g(r)$ of C-H at (a) 200 K and (b) 300 K computed via AIMD simulations for hydrogen storage on HGY [38].

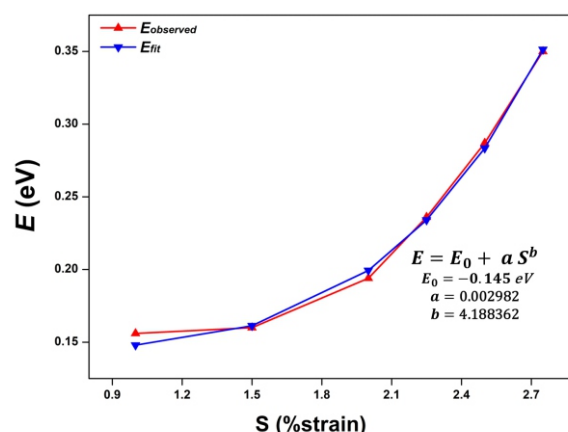


Fig.10: Variation of hydrogen adsorption energy with applied compressive biaxial strain on HGY. The results from the present simulation are compared with that of empirical fitting and the fitting equation and constants are mentioned inset (bottom-right) [38].

to modify its electronic structure without compromising on its structural stability. Applying compressive strain in nanomaterials causes an increase in charge density in the π molecular orbitals of carbon-based 2D nanomaterials. This, in turn, increases the orbitals' polarisation, which can improve their hydrogen affinity for hydrogen over that of pristine carbon-based nanomaterials. Here we describe the design of few light element based 2D materials for enhanced hydrogen storage, adopting the strain engineering technique.

Strain Engineering in 2D holey graphene (HGY)

Herein, the interaction of hydrogen with pristine and strained 2D holey graphene (HGY) has been examined. Upon subjecting HGY to biaxial compressive strain (1%–2%), linear compression of C-C bonds was noted and beyond 3% strain the structure distorted. Hydrogen adsorption on strained HGY showed enhanced adsorption energies compared to pristine HGY, peaking at -0.350 eV for 2.75% strain [38].

Based on our investigations, pristine HGY interacted with H_2 via weak van der Waals interactions, evidenced by low adsorption energies. However, under the influence of compressive strain, its electronic properties were altered and a spatial confinement was induced within HGY. The resulting increased charge polarization led to the development of an

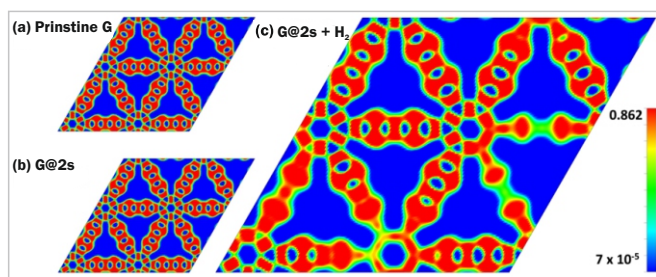


Fig.11: Electron localization function plots of (a) pristine graphdiyne, (b) G@2S, and (c) G@2S + H₂. The color legend is shown inset (bottom right)

electric field within the system, which enhanced the van der Waals interactions of the substrate with H₂. Mechanistic insights revealed that hydrogen adsorption on strained HGY occurs via an assisted van der Waals interaction mechanism. This interaction was most pronounced at 2% strain, where the work function analysis indicated increased conductivity and maximum interaction with hydrogen molecules. Furthermore, applied strain of 2.75% resulted in the highest hydrogen adsorption energy, significantly improving storage capacity. The gravimetric uptake of H₂ in 2.75% strained HGY was 5.88 wt% computed under the DFT conditions of 0 K and no applied pressure, satisfying the 2025 US DOE target for solid-state H₂ storage in light vehicles. The influence of temperature and pressure conditions on hydrogen retention by the substrate was evaluated; vapour pressure calculations revealed that at 50 bar, hydrogen delivery could occur at 342 K. The thermal stability of the strained HGY was confirmed through AIMD simulations, ensuring its viability for practical hydrogen storage applications. The first $g(r)$ peak was noted at ~ 4.7 Å as shown in Fig.9, consistent with weak interactions between H₂ and strained HGY. Fig.10 displays the variation of adsorption energy of H₂ with the strain, fitted with an empirical formula. Thus, our findings highlight strain engineering as a promising pathway to enhance hydrogen storage in carbon nanomaterials like HGY, offering a feasible solution that avoids the limitations of metal-based approaches.

Strain Engineering in 2D graphdiyne

We have investigated the possibility of compressive strain application of synthesized 2D graphdiyne [39], an advanced member of graphene family. Under the influence of 2%

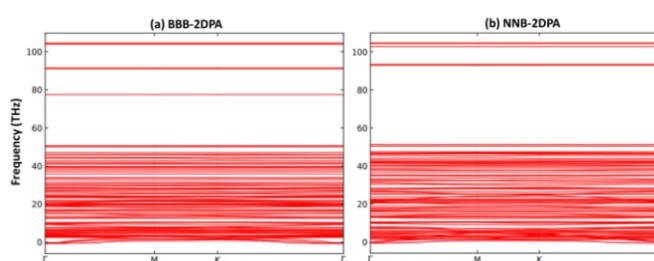


Fig.12: Phonon dispersion curves for (a) BBB-2DPA and (b) NNB-2DPA; absence of negative frequency confirms dynamic stability [42].

compressive biaxial strain (G@2S), the adsorption energy of hydrogen on graphdiyne improves to -0.224 eV/H₂ with a maximum predicted gravimetric capacity of 6.942 wt%. The mechanism of binding may be via an enhanced physisorption owing to the altered electronic structure of graphdiyne under the influence of strain. The strained system is mechanically stable at 300 K as verified by molecular dynamics simulations [40].

The electron localization function plots for graphdiyne, G@2S, and G@2S + H₂ (Fig.11) shows that the binding of hydrogen is accompanied by a reduction in local electron density near neighboring acetylenic bonds (green regions), and the C6 ring shows increased electron density (enhanced red regions). Thus, the binding interaction of hydrogen with G@2S may be due to an enhanced physisorption owing to the modified electronic structure under applied strain. Hydrogen storage in G@2S may be reversible as hydrogen vapor pressures of 12 bar can be achieved at 290 K. Based on our predictions, strain engineering in graphdiyne can be explored in experimental trials for potential hydrogen storage applications.

Strain Engineering in 2D graphene

We also reported through DFT simulations that in a 4×4 supercell of graphene, the application of 6% biaxial strain led to a gravimetric hydrogen uptake of 9.4% with an average adsorption energy of -0.42 eV/H₂ [41]; the enhanced hydrogen storage capacity of strained graphene was attributed to altered electronic properties of graphene under strain, leading to an enhanced charge transfer interaction between the substrate and hydrogen.

Table 2: Hydrogen adsorption energies, H-H bond length, and shortest distance between H and the substrate for the adsorbed H₂ in the doped 2DPA systems. The best performing systems are formatted in blue[42].

System	Ead (eV)	Distance or bond length (Å)	
		H-H	Substrate-H
Pristine 2DPA	-0.116	0.75 (isolated H ₂)	–
N-2DPA	-0.162	0.753	2.887
NN-2DPA	-0.168	0.753	2.550
NNN-2DPA	-0.161	0.752	2.963
B-2DPA	-0.155	0.753	2.717
BB-2DPA	-0.224	0.756	2.474
BBB-2DPA	-0.234	0.757	2.053
BN-2DPA	-0.179	0.752	2.947
BBN-2DPA	-0.170	0.754	2.694
NNB-2DPA	-0.268	0.757	2.064



Non-metal Substitution

Substitutional doping with light elements such as B and N, which are similar in size to C, can lead to hole (B) or electron (N) doping in the host material. The increased conductivity of charge carriers brought about by B/N doping can enhance the substrate's interaction with hydrogen.

Non-metal Substitution in 2DPA nanosheet

We have also demonstrated the potential of non-metal substitutional doping in 2DPA as a viable strategy for enhancing its hydrogen affinity and therefore its potential towards hydrogen storage applications without the need for metal adatoms; metal adatoms cause decreased gravimetric uptakes and poor efficiency over time owing to the high likelihood of metal-clustering. A systematic doping protocol was established and B- and N-doping configurations were identified by selectively doping in a manner so as to improve the H_2 affinity of the substrate. The BBB- and NNB-2DPA systems exhibited optimal hydrogen adsorption energies within the DOE's prescribed range and showed improved H_2 -substrate interaction strength brought about by polarization-assisted van der Waals forces. B/N doping led to modifications in the electronic structure and conductivity and brought about charge polarization. This in turn improved the substrate's H_2 affinity via an assisted physisorption route. The first hydrogen adsorption energy in BBB- and NNB-2DPA was considerably enhanced (-0.234 and -0.268 eV, respectively) as compared to that in pristine 2DPA (-0.116 eV) [42]. Table.2 displays the adsorption energy on various configurations obtained by N/N substitution on 2DPA. Thermal stability studies using AIMD simulations and phonon dispersion analysis (Fig.12) confirmed the robustness of BBB- and NNB-2DPA at room temperature, making these systems viable for practical applications. The gravimetric hydrogen uptake of these substrates was found to be promising, with 4.778 wt% and 4.040 wt% obtained for BBB- and NNB-doped 2DPA, respectively. Vapour pressure calculations for a delivery pressure of 12 bar revealed desorption temperatures of 252.186 K and 275.91 K for BBB- and NNB-decorated 2DPA, respectively.

Non-metal Substitution in 2DPA nano-sheet Graphdiyne (GDY)

We have also theoretically explored the hydrogen storage capability of graphdiyne (GDY) which is an advanced member of 2D graphene family and has been synthesized. Nitrogen and boron doped graphdiyne (BCN-GDY) have also been demonstrated for hydrogen storage. Although pristine GDY exhibits weak hydrogen adsorption, strategic B/N co-doping induces charge redistribution and polarization of H_2 molecules, yielding enhanced physisorption which significantly improves its hydrogen storage capacity. BCN-GDY achieved a remarkable hydrogen weight percentage of 14.29%, which is well above the DOE target of 6.5 wt%, with an average adsorption energy of -0.23 eV/ H_2 , which falls within the optimal range of -0.2 to -0.7 eV/ H_2 [43]. The dehydrogenation temperature range is 256–331 K at 5 bar, room temperature. Overall, BCN-GDY emerges as a highly promising material for hydrogen storage applications, with superior adsorption/desorption kinetics and substantial hydrogen capacity, positioning it as a strong candidate for clean energy technologies.

Conclusions

This article uses Density Functional Theory (DFT) to investigate the interaction, charge transfer mechanisms, and hydrogen storage capacity of transition metal-decorated 2D carbon nanostructures (2D polyaramid, holey graphyne, biphenylene). The effect of strain on 2D materials for enhancing the hydrogen storage capability has also been addressed. Few systems, e.g. Ti and Zr doped 2D polyaramid, Niobium doped biphenylene and strained holey graphyne have been identified as promising materials to experimentally fabricate 2D material based hydrogen absorbing materials for next generation hydrogen storage devices.

Acknowledgments

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Research Highlights

लिथियम-पेग्माटाइट अयरस्क प्रक्रम-अपशिष्ट से रुबिडियम, सीज़ियम और पोटैशियम का निक्षालन द्वारा प्रतिप्राप्ति

लिथियम-युक्त पेग्माटाइट प्रसंस्करण अपशिष्ट का मूल्यवर्धन

Leach Recovery of Rubidium, Caesium and Potassium from a Lithium-Pegmatite Ore Process Residue

Value Addition to Lithium-Bearing Pegmatite Processing Residue

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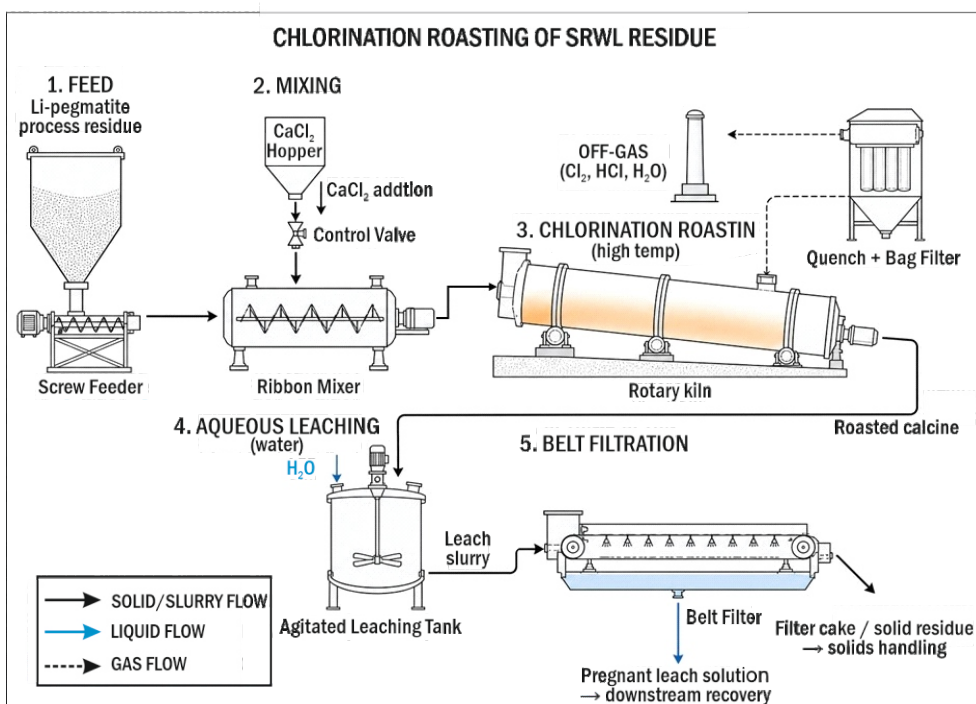
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Rubidium (Rb) and caesium (Cs) are strategically important metals used in atomic clocks, night-vision systems and aerospace technologies. Potassium (K), in contrast, is consumed on a much larger scale, predominantly in the fertilizer sector. India's dependence on imported potash highlights the importance of developing indigenous K resources and recovering associated Rb and Cs from a process residues enriched in these metals. In the present study, a sulphation-roasted-water-leached residue of lithium-bearing pegmatite ore was investigated as a secondary source of these alkali metals. The material contained 0.41 wt% Rb, 0.11 wt% Cs and 4.14 wt% K, principally hosted in microcline, leucite and nepheline. A chlorination roasting-water leaching route using calcium chloride dihydrate ($\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$) was developed to convert these framework-bound alkali metals into water-soluble chlorides.

Chlorination of the alkali-bearing aluminosilicate phases by addition of calcium chloride is found thermodynamically favorable, with the driving force increasing with temperature. Process parameter optimization studies showed that above a critical dosage, hydrolysis of calcium chloride promotes wollastonite formation by reacting with silica, reducing the amount of chlorinating reagent available for alkali-metal extraction and yielding only marginal additional gains. X-ray diffraction confirmed the transformation of the alkali-bearing phases and the formation of calcium aluminosilicate and calcium silicate products. Maximum leachabilities of 95% Rb, 93% Cs and 87% K were obtained by roasting at elevated temperature using $\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$, followed by plain-water leaching, enabling simultaneous recovery and a basis for selective separation. The findings support indigenous resource development and improved supply-chain security of the strategically important alkali metals.



Schematic representation of calcium chloride dihydrate assisted chlorination of alkali bearing aluminosilicates to form water soluble Rb, Cs and K chlorides [1].

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उच्च-एंट्रॉपी बोराइड

अति-उच्च तापमान वाले सिरेमिक पदार्थों का एक नया वर्ग

High-Entropy Borides

A new class of ultra-high-temperature ceramics

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High-entropy borides (HEBs) are a class of multi-principal-element ultra-high-temperature ceramics (UHTCs) in which multiple transition metals occupy the metal sublattice of a diboride structure, typically forming a hexagonal AlB-type solid solution. Their distorted lattice can promote high configurational entropy, leading to distinctive combinations of mechanical properties like high hardness, thermal stability, oxidation resistance. These characteristics have attracted considerable interest in HEBs for demanding applications such as high-temperature structural components, hypersonic systems, and energy systems.

In the present study, Equiatomic (Ti . Nb . Ta . Hf . Zr .)B and non-equiatomic (Ti . Nb . Ta . Hf . Zr .)B high entropy borides were synthesized via boro/carbothermal reduction and consolidated by hot pressing and spark plasma sintering at 1900 °C. Both compositions formed single phase hexagonal AB solid solutions, as confirmed by diffraction and microscopy. Densification followed Coble creep behaviour, with higher activation energies observed

for hot pressing than spark plasma sintering. Microstructural analysis revealed a largely homogeneous matrix with localized Nb-rich and minor Ta-rich segregations, contributing to limited grain coarsening. The non-equiatom composition showed slightly reduced hardness but improved fracture toughness (~4.1 MPa·m^{1/2}). Hardness ranged from 16 to 23 GPa (Vickers) and up to ~28 GPa by nanoindentation, with elastic modulus reaching ~455 GPa. Flexural strengths of 500–525 MPa were obtained, with fracture dominated by transgranular brittle mechanisms.

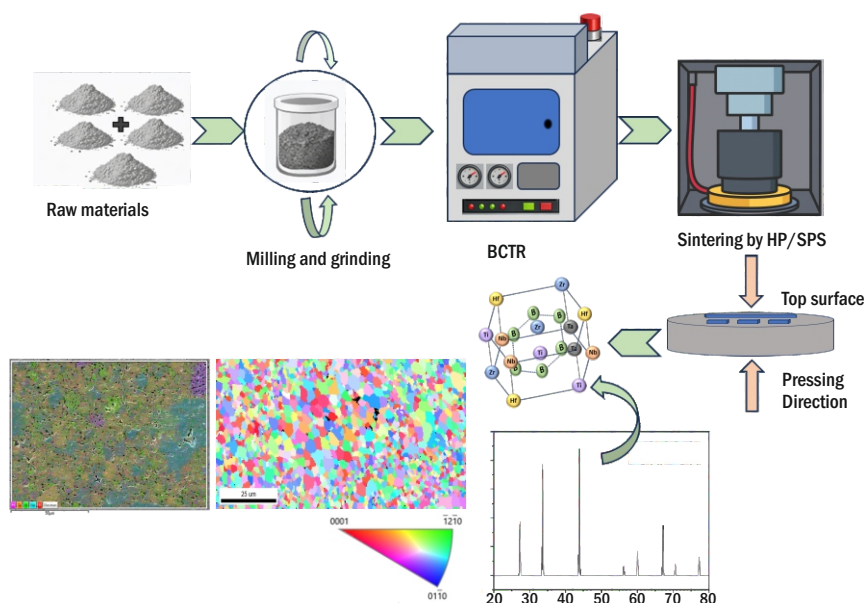
Reference:

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Schematic representation of Synthesis, densification and characterization of High entropy Borides [1].



Research Highlights

जैव-सिरेमिक के पिको सेकंड लेजर टेक्सचरिंग एवं स्पंद लेजर निक्षेपण के माध्यम से Ti6Al4V का बहु-कार्यात्मक सतह संशोधन
उन्नत कार्यात्मकता के लिए **Ti6Al4V** की लेज़र सतह अभियांत्रिकी

Multifunctional Surface Modification of Ti6Al4V through Pico-second Laser Texturing & Pulsed Laser Deposition of Bio-Ceramics *Laser Surface Engineering of Ti6Al4V for Enhanced Functionality*

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Ti64 (Ti6Al4V) is widely used for orthopedic, dental, and cardiovascular implants owing to its high strength, excellent biocompatibility, and corrosion resistance. However, its bio-inert surface limits direct tissue bonding and effective osseointegration, potentially compromising long-term implant stability. Since tissue integration is strongly governed by surface properties, controlled surface engineering offers an effective approach to enhance bioactivity, mechanical interlocking, and implant longevity [1-2]. In our newly published study, we report synergistic effect of two-step surface improvement of Ti6Al4V by picosecond laser surface texturing (LST) followed by pulsed laser deposition (PLD) of two types of ceramics, bio-active 45S5 glass and bio-inert zirconia. The modified hybrid surface (LST + PLD) exhibited altered topography, roughness, and wettability. Electrochemical analysis performed in simulated body fluid revealed improve-ments in corrosion resistance and impedance properties. Biological evaluation included study of U2OS osteosarcoma cells adhesion, proliferation, counts and the antibacterial efficacy of sample surface against

Bacillus gram positive bacteria. The results revealed that, the zirconia coated sample possesses maximum corrosion potential (0.03 V), minimum corrosion current density (1.02×10^{-6} A/cm²) and almost six-fold improvement in antibacterial behavior. In contrast, bio-glass coating exhibited highest cell density (~ 112 cells per 4 mm²) compared to other samples. These finding suggested that, the hybrid approach of laser texturing with bio ceramics coating can synergistically improve functionality of Ti6Al4V, making it a promising candidate for advanced orthopedic and dental implant applications.

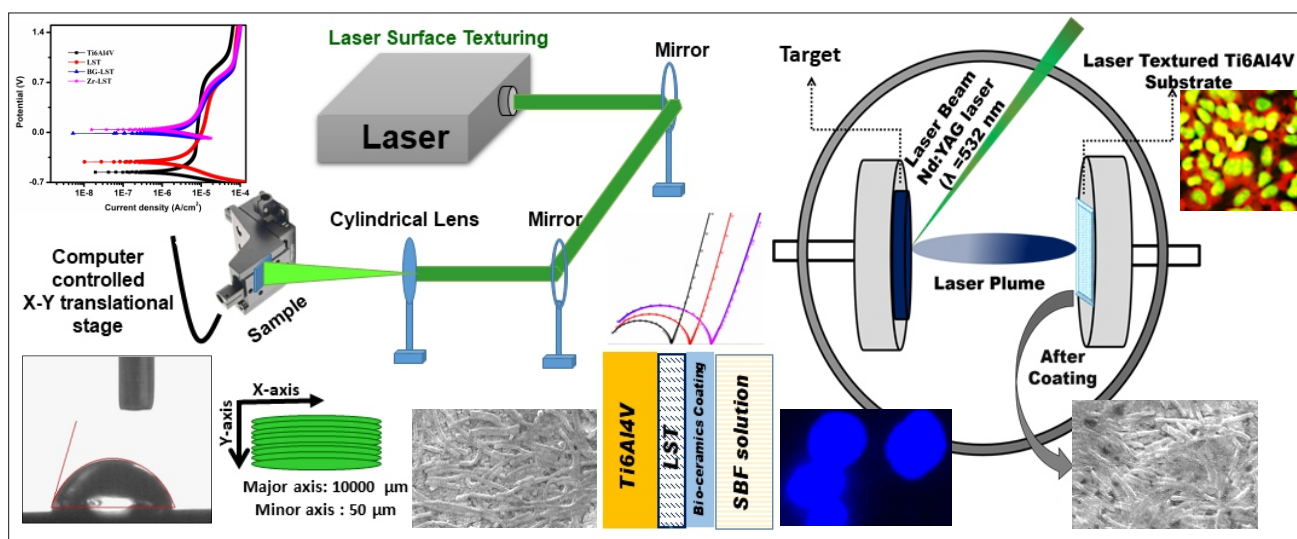
Reference:

- [1] E. Marin, A. Lanzutti, Biomedical applications of Titanium alloys a comprehensive review, Materials 25 (2023) 114.
- [2] A.S. Daniel, A.P.P. Anand, J. Naveen, T. Khan, S.H. Khahro, Advancement in biomedical implant materials—a mini review, Front. Bioeng. Biotechnol. 12 (2024) 1400918.

About the author



Dr. Sunita Kedia is currently working as a Scientific Officer/F at Laser & Plasma Technology Division, Bhabha Atomic Research Centre (BARC), Mumbai, India. Her research focuses on Laser-Material processing, Surface modified biomaterials, Bio-ceramics thin-film coating, and Selective laser sintering. She has about 50 peer-reviewed publications, with 550 citations.



Schematic representation of LST and PLD with relevant results.

Sunita Kedia, Prabha Soundharraj, Rajesh K. Chaurasia, L.V. Panicker, B.K. Sapra, J. Padma Nilaya, "Synergistic effect of picosecond laser texturing and pulsed laser deposition of bio-ceramics on Ti6Al4V performance" Optics and Laser Technology, 203 (2026) 115673.



त्वरित प्रतिदीप्ति-आधारित एल्ब्यूमिन विश्लेषक

गुर्दे के कार्य-विकार से संबंधित एल्ब्यूमिन्यूरिया की शीघ्र पहचान हेतु

Rapid Fluorescence-Based Albumin Analyser

For Early Detection of Albuminuria Associated with Kidney Dysfunction

Prabhat K. Singh¹ and Nitin O. Kawade²

¹Radiation & Photochemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai - 400085, INDIA

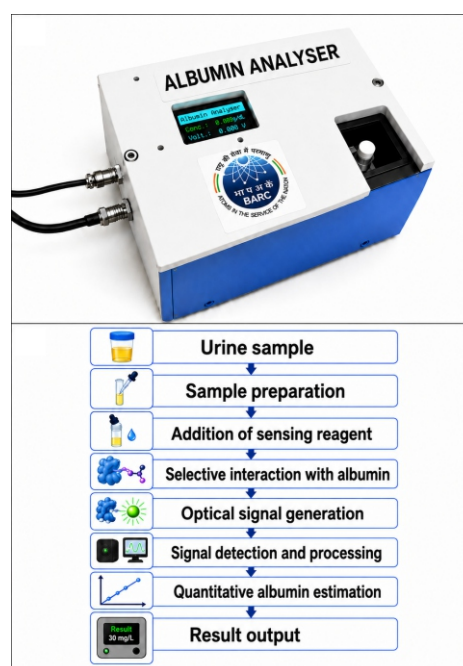
²Laser & Plasma Technology Division, Bhabha Atomic Research Centre, Trombay, Mumbai - 400085, INDIA

Albumin in urine is an important biomarker of renal dysfunction, with increased urinary albumin excretion often appearing before an overt decline in kidney function. In particular, moderately increased albuminuria, traditionally referred to as microalbuminuria, is associated with early renal damage and is also an indicator of increased cardiovascular risk. Sensitive and quantitative determination of urinary albumin therefore has considerable value for early screening and disease monitoring. Conventional approaches for urinary albumin estimation include semi-quantitative dipsticks and quantitative immunochemical techniques such as immunoturbidimetry and immunonephelometry. Although established laboratory methods provide good analytical performance, their dependence on specialised instrumentation, reagents and trained personnel can limit their suitability for rapid and decentralised screening. Dipstick-based methods, on the other hand, are convenient but have limited sensitivity and provide primarily semi-quantitative information.

To address these limitations, an indigenously developed fluorescence-based Albumin Analyser has been designed for rapid and selective quantification of albumin in urine. The sensing strategy employs a water-soluble aggregation-induced emission (AIE) probe which is only weakly fluorescent when molecularly dispersed. In the presence of albumin, the probe molecules aggregate on the protein surface, restricting their intramolecular motion and producing a pronounced fluorescence “turn-on” response. The Albumin Analyser translates this molecular response into a simple quantitative readout. An LED excites the sample contained in a quartz cuvette. The resulting fluorescence is selected using a band-pass filter and detected by a photomultiplier tube (PMT). The optical signal is converted into an electrical voltage whose magnitude is related to the concentration of albumin present in the sample.

A simple background-correction step accounts for variations in the urine matrix, enabling reliable estimation of albumin concentration. The developed system provides a limit of detection of 21 ± 0.3 nM, a linear detection range of 0–0.6 μ M, and a typical response time of 1–2 min. The technology has undergone extensive photophysical and analytical characterisation, and comparison with standard clinical assays and a commercially available microalbumin

kit demonstrated the potential of the platform for reliable urinary albumin analysis. Built using commercially available components and requiring relatively low reagent consumption, the Albumin Analyser represents a promising compact platform for rapid urinary albumin screening and point-of-care renal health assessment, particularly where access to conventional laboratory infrastructure may be limited.



Fluorescence-based Albumin Analyser and schematic workflow.

About the authors



Dr. Prabhat K. Singh is Scientific Officer (G) at the Radiation and Photochemistry Division, BARC, Mumbai. His research focuses on ultrafast spectroscopy, supramolecular chemistry, and self-assembled materials for optical bio- and chemosensing. He has authored about 150 peer-reviewed publications and received several national and international scientific honours.

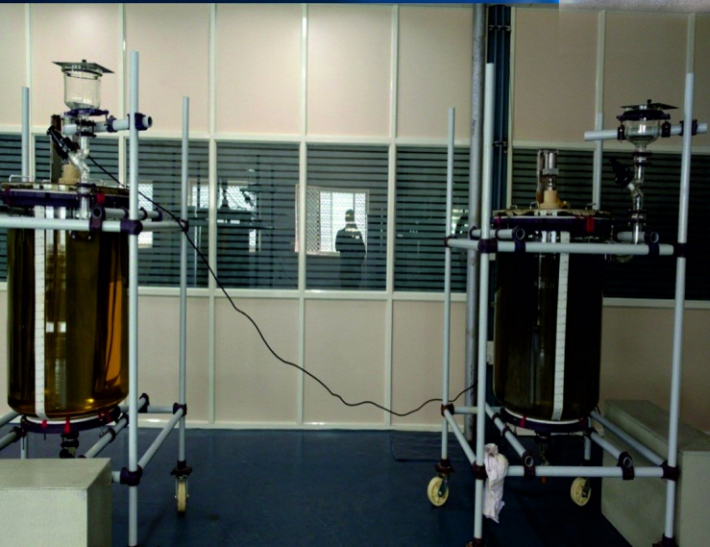
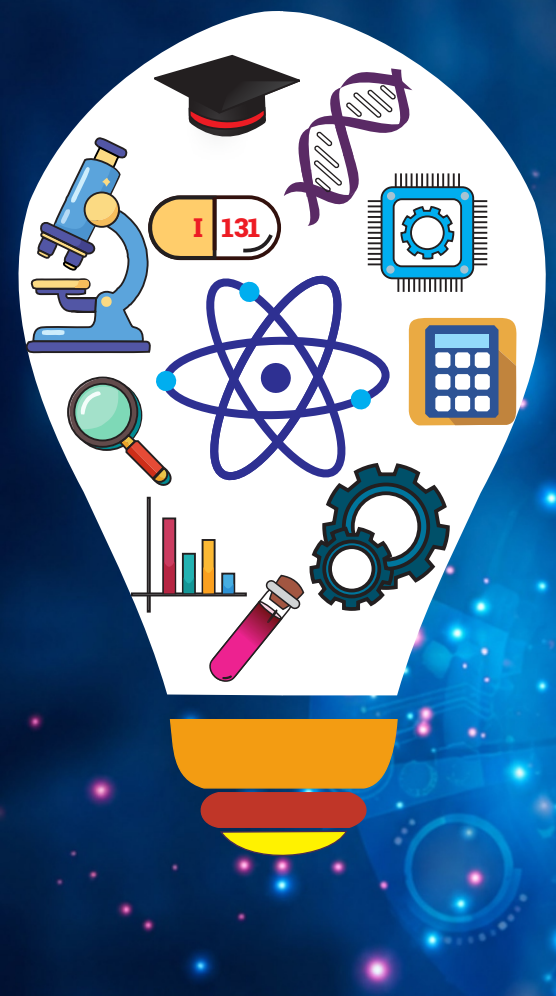


Shri Nitin O. Kawade is Scientific Officer (H) at the Laser and Plasma Technology Division, BARC, Mumbai, and a recognized M.Tech. guide at HBNI. His areas of expertise include laser-based instrumentation, laser control systems, particle image velocimetry, and fibre-optic sensors.



NUCLEAR R&D Tech Spin-offs

Bhabha Atomic Research Centre (BARC) continues to foster industry collaboration by transferring emerging nuclear spin-off technologies and associated know-how besides stimulating rural entrepreneurship. The Centre is also accelerating efforts to incubate deep-tech startups in high-priority domains critical to sustained economic growth.



प्रौद्योगिकी का सुव्यवस्थीकरण एवं हस्तांतरण Technology Streamlining & Transfer



BARC continued to streamline indigenous technologies for public and industrial applications in areas like agriculture, healthcare, metallurgy, quality assurance, and nutrition. During the review period (July-August 2026), three new technologies were placed in the public domain.

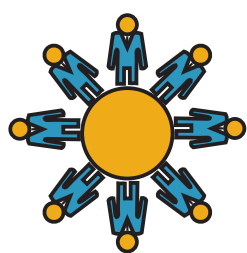


Autonomous Seal Cutting System (EG51DRHR): A compact, modular device for safely opening sealed containers with hazardous materials. It uses a rotary table, a torque-controlled gripper, and a protected cutting unit to ensure precision and prevent container damage. Its small size suits space-limited settings like pharmaceutical units, and it can be operated manually or via a GUI.

Passive Catalytic Recombiner Device (PCRD) (CH52ChD): A safety device that removes hydrogen in closed containments. It uses catalytic plates coated with platinum and palladium to convert hydrogen and air into steam, creating a passive flow that continuously draws in hydrogen-rich gas from the bottom. It is used in nuclear reactors during coolant loss conditions and in other hydrogen gas-using industries.

Gamma Radiation Process for Ready-to-Eat Onions: A combined processing and irradiation method that reduces post-harvest losses and extends the shelf life of fresh, ready-to-eat onions. This helps maintain onion quality for domestic and international markets, benefiting hotels, restaurants, retailers, and traders.

इनक्यूबेशन एवं नवोद्यम पारितंत्र Incubation & Startup Ecosystem



AIC BARC Anushakti Foundation, supported by the Atal Innovation Mission (AIM), kept building the deep tech start-up ecosystem through incubation, tech commercialization, and industry tie-ups. A national Techathon 2.0 cohort by the DAE Incubator Alliance to attract deep tech start-

ups saw 116 applicants. 18 teams were selected across General, Narishakti (women), and Junior categories. AIC Anushakti helped organize and served on screening juries of Techathon 2.0 cohort. M/s. 6C NanoCarb Pvt. Ltd. commercialized its carbon nanotube technology, with a launch event at IIT Bombay Research Park. Programs were held at the University of Mumbai's Nano Science department. The Head of AIC ANUSHAKTI spoke on DAE technology transfer at an event organised by AIC IGCAR FAST Foundation on 24 July 2026. AIC ANUSHAKTI also engaged with AIM, national innovation programs, and DAE leadership to strengthen tech translation and incubation. During the review period four technologies were transferred to industries and six technology transfer agreements were renewed for five more years.

ग्रामीण उद्यमिता Rural Entrepreneurship



AKRUTI Kendras promoted rural entrepreneurship through awareness campaigns, technology demonstrations, trainings, and forging partnerships. Tarapur Kendra hosted entrepreneurs and self-

help groups during the review period. An orientation camp during Ashadhi Wari showcased BARC technologies and development initiatives supported by NPCIL, BARC, and SVERI with Pandharpur as venue. MGU Kendra conducted workshops at four institutions in Kerala, including Caritas College of Pharmacy, Mar Athanasios College, MG University's DLLE, and Union Christian College, Aluva. The AKRUTI Kendra at Jai Hind College was formally opened by Dr. K. N. Vyas, former DAE Secretary and AEC Chairman, and an alumnus of the college. The Head of TT&CD, AKRUTI Group Leader, and students from various faculties attended.



भारत के रक्षा प्रमुख ने अपने
जीवन-परिवर्तनकारी आदर्शों से प्रशिक्षण
विद्यालय के युवा स्नातकों को प्रेरित किया

India's CDS inspires young TS Graduates with his life transforming ideals

General N. S. Raja Subramani graced the annual graduation ceremony as chief guest, commemorating the successful completion of the 69th BARC Training School batch, and addressed the gathering at the Central Complex Auditorium



'D' in determination stands for DISCIPLINE - a bedrock of your life. When we look at a cricketer or a cricket team which has won a medal or won the World Cup or when we see a country or an athlete standing on a podium we only look at that particular moment in time. But that particular moment of time has arrived because of immense discipline, practice and hardwork that was put in to reach that goal. Discipline will ensure that you are mentally and physically fit, able to carry on and reach goals you aspire to...

It means EVOLVE. The world is rapidly changing. Technology is moving at a breathtaking pace. Each one of us have to cultivate the habit of evolving, adapting, having curiosity, and habit of life-long learning. Your learning does not stop. Today, you have graduated. Learning begins and continues till you continue on this earth. You have to be a life-long learner who's curious - who takes initiatives - who's a problem solver, not a problem giver. Get into the habit of seeing how you can come up with solutions to a problem either it be in your field or in other fields. You may not have all the knowledge that is possible but if you can think logically you can come to reasonable solutions to whatever problems you face...

Learn to be like a TIGER. What does a TIGER do? He is patient - he is resilient - he keeps quiet till he sees his prey on whom he pounces and he is able to execute the kill in one go. Emulate yourself on that. Be fearless, have focus, have the ability to take risk and a single-minded determination to get the job done...

Empathy is important in all stages of life. It is the ability to stand in others' shoes. Whether it be a friend, whether it be a subordinate, Whether it be a superior. That is the bedrock of trust - That is the bedrock of collaboration - That is the bedrock of teamwork. Cultivate this habit...

Respect yourself. Respect time. Learn to manage time. When I was young I had a commanding officer who I always used to notice that his table was absolutely clear. And, I used to be working all the time. I asked him once I seem to be working all the time and you seem to be free. He said: "Son, please listen carefully. Please spend two-thirds of your time planning for the future and one-third of your time in the present." What does it mean? All of us are happy to do routine mundane jobs. We don't spend time in thinking and planning. If you put adequate time in thinking and planning, automatically you will spend less time in the present...

M means ME. Invest in yourself. Be confident. You are unique in this world. Nobody else is going to live your life. Nobody else is going to know what you are going to do. So, therefore each one of you should have confidence in your abilities. You need not compare what the other person is doing. It does not matter where you start...

Integrity is a quality that I as a leader value the most in my subordinates. In nuclear, there's no compromise on safety. Manipulation of data or not telling the correct thing at the right time may lead to potential mishaps in the future. Therefore, value integrity. Taking short-cuts may give you gains in the short term. But take it from me, integrity is what is the bedrock of success in the long term...

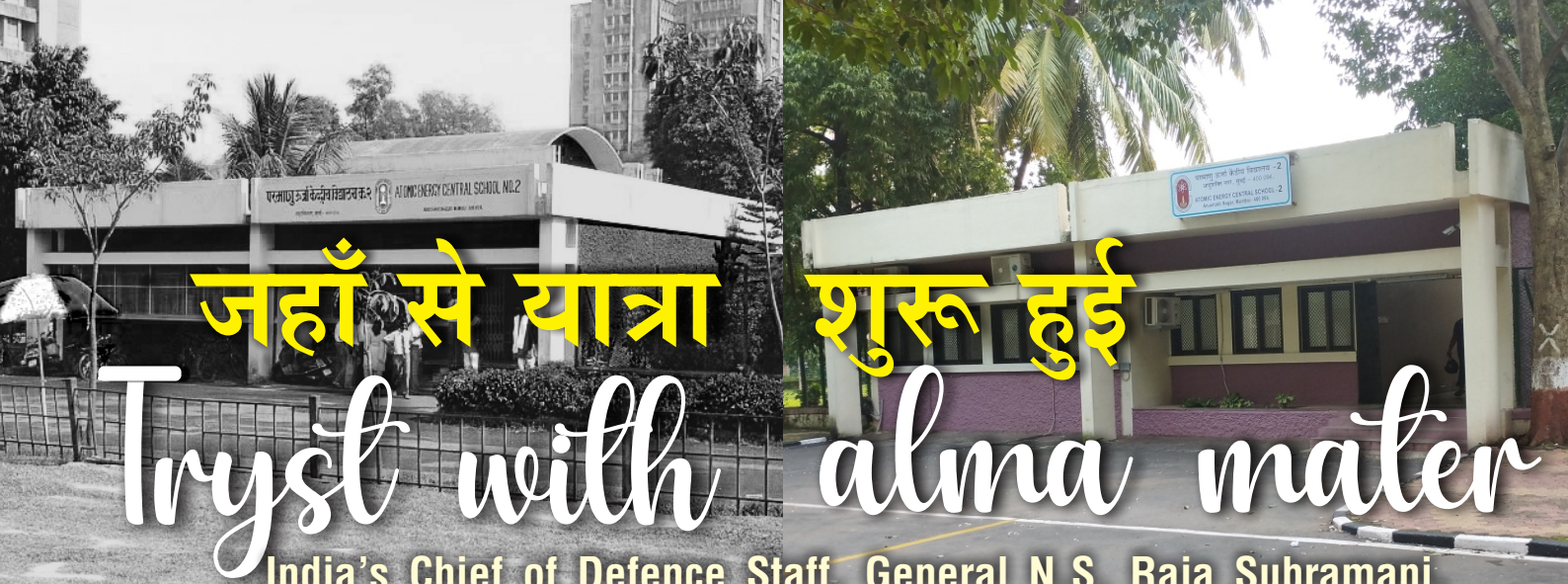
D. E. T. E. R. M. I. NATION

SELF RELIANCE

BARC and your predecessors have ensured that India is fully self reliant in nuclear fuel cycle; and in our ability to build reactors; and in our ability to generate electric power through nuclear means. We need to build upon self-reliance. Self-reliance does not mean isolation - It means being confident in our capabilities - It means being able to innovate - It means being able to stride confidently, have confidence in our capabilities, and have confidence in our ability to shape the future.

TEAMWORK

It is a very important aspect - The ability to work unitedly, collaborate, build upon each others strengths. Synergising and harmonising all our energies is what that will lead us to a glorious future ... When the term 'Buddha Smiled' was coined in 1974, that is the first peaceful atomic test ... We were cut-off from all scientific knowledge and equipment of the world. Our scientists worked and designed our own equipment, worked on our own knowledge, ensured that despite denied all facilities, we could progress ahead and build and shape our own future. Technological excellence alone is not enough. It has to be backed up by ethical leadership.



जहाँ से यात्रा शुरू हुई Tryst with alma mater

India's Chief of Defence Staff, General N.S. Raja Subramani, visits Atomic Energy Central School, recalls childhood memories



*It is 50 years
since I have returned to Anushakti Nagar.*

*My father was an employee of DAE. He was working as a
civil engineer in the late 1960s (I think in '69 or '70). He served here
(in BARC) and then moved to Narora, and later to Kalpakkam where he
was involved in the construction of reactors. If I remember correctly,
he was also the civil-engineer-in-charge for the Fast
Breeder Test Reactor in Kalpakkam.*

*I've done
my schooling in Atomic Energy
Central School here in Mumbai where I
studied till Class VI and I did my remaining
schooling in Narora till Class XI before joining
the National Defence Academy.*

*I was
preparing for IIT and my father
told me that go and prepare for this exam (NDA).
This will be a test for you, and a preparation for you for
IIT. So, I prepared and I passed. At that time you could join
NDA without doing Class XII. Little did I realise that you have
to study life-long to reach where you are now. And this
applies to every profession, and it is also a
good lesson for you.*





ट्रॉम्बे वार्तालाप

जुलाई-अगस्त '26

Trombay Colloquia

Jul-Aug '26



Future is Incredibly Exciting at CERN

What Next at CERN?

- What is the unknown 95% of universe's mass?
- Why it is made only of matter with hardly any anti-matter?
- Does Higgs Boson interact with the Dark Matter?
- Is Higgs Boson a fundamental particle?
- Why is gravity so weak?

Big Projects

- Future Circular Collider (FCC)-91 km ring
- Capital Outlay: 15 billion Swiss Francs
- Targeted year of operations: 2045-48

Recent Achievements

- For the Large Hadron Collider, 2025 was a record-breaking year
- ATLAS & CMS data for 2025 stands at 125fb^{-1} ; Total so far is 520fb^{-1}
- There's a profound discovery in every 5 years at CERN
- Publications on LHS Experiments reached ~ 4000
- 1500 petabytes of CERN data stored world-wide

Prof. Thomson's visit to BARC, Mumbai on August 31, 2026 was second during his career and first after he assumed charge as CERN's Director General in January 2026. He delivered a talk entitled 'Particle Physics - Today & Tomorrow' at Trombay Colloquium.

Professor Mark Thomson
Director General
European Organisation for Nuclear Research (CERN)

2026

08
July

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50 Years of Solar in India *Achievements and Challenges*

India's Solar Future Bright

2026 is the golden jubilee year for Solar Energy in India

The country will be 2nd/3rd largest deployer of solar energy capacity globally in the next decade

On track to meet COP26 target of having 50% electrical capacity for non-fossil sources by 2030

Deployment Challenges & Potential Threats

Land availability and acquisition can be a problem

Solar needs 5-7 acre per MW

Module deployment takes 12-18 months whereas transmission, line planning & execution takes 3-5 years

Cyber security of solar grid is an interesting area of study.

One way to overcome this potential problem is to manufacture more locally with in-house technology

Prof. Juzer Vasi
Professor Emeritus
IIT Bombay

LIGO-India

*The First AI controlled, quantum enhanced
Gravitational Wave Detector*

LIGO and India

International LIGO draws significant advantages from adding India to the detector network

LIGO Global Network of Detectors : 2 in the US, one each in Italy, Japan and India

LIGO-India Phase I slated for completion in 2033

Hard Scientific Problems in LIGO-India

The technology of ultra-high vacuum tubes functioning at 10⁻⁹ mbar is non-existent in India

Ultra-low noise interferometry expertise for measurement exists only in select S&T communities

People who could do this is not even handful

Prof. Rana Adhikari
Professor of Physics
California Institute of Technology, USA

2026

22
July

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परमाणु ऊर्जा के माध्यम से
तारापुर समुदायों ने
मैत्री संबंधों को किया सुदृढ़

Tarapur Communities Cement Bonds of Friendship over Nuclear Energy

By Nuclear Recycle Board, BARC and SIRD Newsletter Editorial Team, BARC.

The households of six villages in Tarapur, located in the vicinity of Nuclear Recycle Board, BARC and NPCIL units, toured and interacted with senior officials and personnel of the twin nuclear facilities during a full-day public awareness programme held on August 8, 2026.

Around 350 residents from villages in close proximity to Tarapur - Dandi, Ucheli, Unbhat, Ghivali, Savarai and Kamode - enthusiastically participated in the event held at the Community Hall of BARC Colony, Tarapur. The programme served as an ideal platform to familiarise the participants with the significance of nuclear energy activities in the overall development of the country and their contribution towards achieving the long-term vision of Viksit Bharat by 2047.

The participants benefited from a series of tailor-made lectures delivered by experienced speakers on a range of topics, including the importance of nuclear energy, the nuclear fuel cycle, safety, nuclear waste management, health monitoring in nuclear facilities, and the

prevention of serious ailments, including cancer, in day-to-day life. The Mumbai-headquartered Tata Memorial Centre also set up a small exhibition for the benefit of the participants. An edutainment skit titled 'RIGHT CLICK', centred on nuclear energy activities, was written, directed and enacted by the staff of NRB, BARC stationed at Tarapur.

The participants expressed satisfaction that their apprehensions and misconceptions relating to radiation and nuclear facilities were dispelled through their participation in the programme. They also appreciated the opportunity to have their queries on nuclear energy addressed by senior officials during the Q&A session.

The programme was graced by Mr. A. K. Bhole, Site Director, Tarapur Maharashtra Site, NPCIL, and Mr. Ashu Singhal, Commandant, CISF, along with senior officials from BARC, NPCIL and CISF. Program was conducted by NRB, BARC, Tarapur unit. Mr. D.B. Sathe, Director, GSO, BARC, Tarapur welcomed all the participants and guests. Mrs. Mitun Dey, AGM(T), HR, NRB, BARC coordinated the event.

नेत्र दृष्टि का आश्वासन @भा.प.अ. केंद्र Ru-106 नेत्र प्लॉक

Assuring Eye Vision @BARC Ru-106 Plaque



NATIONAL WORKSHOP Ru Plaque Brachytherapy For Treatment of Eye Cancer

August 08, 2026
Multipurpose Hall, TSH, Anushaktinagar

Organised by
Nuclear Recycle Group
Bhabha Atomic Research Centre, Mumbai



By Nuclear Recycle Group and SIRD Newsletter Editorial Team

The Nuclear Recycle Group organized a first-of-its-kind **national workshop** on Ru Plaque Brachytherapy for Eye Cancer Treatment to commemorate seven successful years of brachytherapy using BARC-developed Ru-106 plaque for treatment of eye cancers in India. Mr. Vivek Bhasin, Director, BARC inaugurated the one-day workshop on August 8, 2026 in the Multipurpose Hall at Anushakti Nagar. Experts from BARC, leading ophthalmic oncology centres, AIIMS New Delhi, corporate hospitals, the Army Hospital, Dr. Shroff's Charity Eye Hospital, AERB and BRIT converged at the workshop, providing a multidisciplinary platform for deliberations on ocular plaque brachytherapy. Eminent ophthalmologists shared their experience with plaque brachytherapy, including current indications and outcomes, long-term clinical experience, and the adoption of BARC-developed plaques at various leading eye-care institutions. The dosimetric characterization of BARC Ru-106 eye plaques, plaque simulation tools developed by BARC, and comparative experience with imported and indigenous plaques also became part of the deliberations. The programme concluded with a panel discussion involving experts from BARC, BRIT, AERB and the ophthalmic oncology community, providing an opportunity to deliberate on the clinical, technical, regulatory and implementation aspects of ocular plaque brachytherapy and to identify avenues for its wider and safe adoption.

भाभा परमाणु अनुसंधान केंद्र, मुंबई में पुष्पित एवं पल्लवित होती राजभाषा

Rajbhasha (Official Language)
Flourishing and Thriving in BARC



भाभा परमाणु अनुसंधान केंद्र, मुंबई में राजभाषा के प्रभावी कार्यान्वयन के अंतर्गत जुलाई-अगस्त, 2026 के दौरान राजभाषा तिमाही प्रगति रिपोर्ट भरने वाले पदाधिकारियों हेतु परिचर्चा कार्यक्रम, राजभाषा के प्रगामी प्रयोग हेतु प्रशासनिक अधिकारियों के साथ बैठक, केंद्र की हिंदी वैज्ञानिक पत्रिका 'परमाणु विज्ञान' के द्वितीय अंक के प्रकाशन हेतु संपादकीय समिति की बैठक, केंद्र में राजभाषा के प्रचार प्रसार को गति प्रदान करने हेतु भा. प. अ केंद्र राजभाषा समन्वय समिति की बैठकें एवं अन्य गतिविधियां आयोजित की गईं:

राजभाषा तिमाही प्रगति रिपोर्ट भरने पर परिचर्चा कार्यक्रम : राजभाषा कार्यान्वयन समिति की बैठक में लिए गए निर्णय के अनुसार, दिनांक 06 जुलाई '26 और दिनांक 15 जुलाई '26 को प्रशासन, लेखा, सुरक्षा आदि अनुभागों में राजभाषा तिमाही प्रगति रिपोर्ट भरने वाले पदाधिकारियों हेतु विशेष परिचर्चा कार्यक्रम का आयोजन किया गया जिसमें क्रमशः 49 और 11 पदाधिकारियों ने प्रतिभागिता की। दो सत्रों में आयोजित इस परिचर्चा कार्यक्रम में राजभाषा तिमाही प्रगति रिपोर्ट के महत्व पर प्रकाश डालते हुए इसके प्रत्येक मद की विस्तृत चर्चा की गई और प्रतिभागियों की शंकाओं का समाधान किया गया।

राजभाषा के प्रगामी प्रयोग हेतु प्रशासनिक अधिकारियों के साथ बैठक : कार्मिक प्रभाग के विभिन्न अनुभागों में किए गए राजभाषा कार्यान्वयन की स्थिति के निरीक्षण के पश्चात क्रमिक विकास को ध्यान में रखते हुए प्रशासनिक अनुभागों के अधिकारियों के साथ दिनांक 12 अगस्त '26 को एच.आर.डी. हॉल, सी.सी. में बैठक का आयोजन किया गया।

श्री मनोज सिंह, अध्यक्ष, आंतरिक राजभाषा निरीक्षण समिति की अध्यक्षता में आयोजित इस बैठक में श्री डी. श्रीनिवास राव, मुख्य प्रशासनिक अधिकारी ने प्रशासन का नेतृत्व किया। इस बैठक में, आंतरिक राजभाषा निरीक्षण समितियों के संयोजकगण, सदस्यगण, उप-स्थापना अधिकारीगण, सहायक कार्मिक अधिकारीगण इत्यादि उपस्थित रहे।

'परमाणु विज्ञान' के संपादकीय समिति की बैठक : डॉ. ए.के. दुरेजा, सह निदेशक, ज्ञान प्रबंधन वर्ग की अध्यक्षता में, हिंदी वैज्ञानिक पत्रिका 'परमाणु विज्ञान' के संपादकीय समिति की बैठक दिनांक 09 जुलाई '26, एच.आर.डी.डी. सम्मेलन कक्ष, अणुशक्तिनगर में आयोजित की गई। इस बैठक में, द्वितीय अंक के प्रकाशन हेतु लेख इत्यादि को अंतिम रूप दिया गया।



वैज्ञानिक अधिकारियों हेतु एक-दिवसीय हिंदी कार्यशाला : राजभाषा के प्रचार एवं प्रसार के अंतर्गत जुलाई - सितंबर '26 तिमाही के लिए दिनांक 21 अगस्त '26 को एस.सी.एफ. ऑडिटोरियम में विभिन्न प्रभागों/अनुभागों में कार्यरत वैज्ञानिक अधिकारियों के लिए एक दिवसीय हिंदी कार्यशाला का आयोजन किया गया। इस कार्यशाला में उपस्थित 52 वैज्ञानिक अधिकारी-डी को राजभाषा नीति, हिंदी टिप्पण एवं आलेखन और अभ्यास, फोनेटिक हिंदी टंकण, प.ऊ.वि. राजभाषा प्रोत्साहन योजना (अटॉलिस), अनुवाद टूल 'अनुवादक' का डेमो, बीटीएस पर राजभाषा कार्यान्वयन से संबंधित सहायक सामग्रियों की जानकारी प्रदान की गई।

भा.प.अ. केंद्र राजभाषा समन्वय समिति की बैठकें : डॉ. जी. सुग्रीलाल, निदेशक, एन.आर.जी. एवं अध्यक्ष, भा.प.अ. केंद्र राजभाषा समन्वय समिति की अध्यक्षता में दिनांक 13 जुलाई '26 को एच.आर.डी. सम्मेलन कक्ष, सी.सी. में समिति की बैठक आयोजित की गई। इस बैठक में, समिति द्वारा आगामी तिमाही में प्रस्तावित कार्यक्रमों के आयोजन पर चर्चा की गई और तत्संबंधी निर्णय लिए गए। इसके अतिरिक्त, दिनांक 31 अगस्त '26 को भी समिति की बैठक आयोजित की गई जिसमें आगामी हिंदी माह '26 के आयोजन से संबंधित निर्णय लिए गए।

राजभाषा की विविध गतिविधियां :

- केंद्र में, मूल रूप से हिंदी में कार्य करने वाले पदाधिकारियों को प्रोत्साहित करने के उद्देश्य से लागू पऊवि राजभाषा प्रोत्साहन योजना (अटॉलिस) के अंतर्गत अप्रैल-जून '26 की तिमाही में कुल 58 पदाधिकारियों ने अपना दावा प्रस्तुत किया।
- केंद्र के अनुभागों/प्रभागों से प्राप्त अप्रैल-जून '26 हेतु तिमाही प्रगति रिपोर्ट की समीक्षा कर संबंधित अनुभागों/प्रभागों को भेजी गई।
- हिंदी अनुभाग, भा.प.अ. केंद्र, मुंबई में दिनांक 25 अगस्त '26 से हिंदी टंकण प्रशिक्षण की कक्षाएं संचालित की जा रही हैं जिनमें 30 प्रशिक्षणार्थी नियमित प्रशिक्षण प्राप्त कर रहे हैं।

राजभाषा के क्षेत्र में पुरस्कार एवं सम्मान : नगर राजभाषा कार्यान्वयन समिति, ठाणे के तत्वावधान में आयोजित 'हिंदी लेख प्रतियोगिता' (विषय : संयुक्त परिवार) में, (i) श्री कुलवंत सिंह, वैज्ञानिक अधिकारी-एच, एम.एस.डी., भा.प.अ. केंद्र, मुंबई को तृतीय पुरस्कार और (ii) श्री जितेश कुमार धमीजा, वैज्ञानिक अधिकारी-ई, सी.एस.डी., ई.एस.जी., भा.प.अ. केंद्र, मुंबई को प्रोत्साहन पुरस्कार से सम्मानित किया गया। दोनों पुरस्कार विजेताओं को हार्दिक बधाई।



Obituary

स्मरणांजलि: डॉ. आर. के. गर्ग (1930-2026)

नाभिकीय पदार्थों के विकास में अग्रणी योगदान देने वाले
रासायनिक अभियंता

In memoriam: Dr. R. K. Garg (1930-2026)

A chemical engineer who made pioneering contributions to nuclear materials development

Dr. R.K. Garg joined Department of Atomic Energy (DAE) in 1956 and was part of the team that was constituted for setting up and commissioning the Uranium Metal Plant in Atomic Energy Establishment Trombay (AEET), which produced India's maiden uranium metal ingot of nuclear purity in 1959. AEET was rechristened as BARC in 1967.

In a distinguished career spanning around four decades, Dr. Garg played a key role in the indigenous development of front-end nuclear materials, including uranium, zirconium, thorium, rare earths, and subsequently establishing industrial plants for their production. All these developments led to successful deployment of PHWR fleet pan-India.

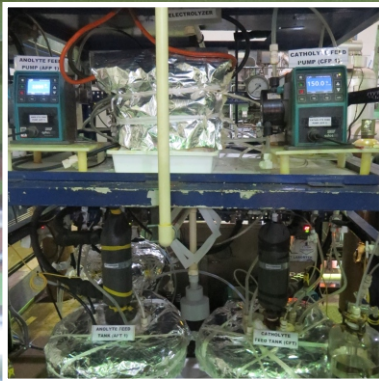
Dr. Garg was integral to the core team that instrumentalised Uranium Enrichment Programme in DAE. Considered to be a highly daunting programme, he guided it with unflinching dedication and foresight. His extraordinary leadership qualities contributed significantly to the development of this technology from scratch to successful plant-scale demonstration.

In Bhabha Atomic Research Centre (BARC), he rose to the rank of the Director of Chemical Engineering Group. Prior to his superannuation in 1990, he served for four years as the Chairman and Managing Director of Indian Rare Earths Limited (IREL). Dr. Garg also authored a book entitled *The Story Of Uranium In India* jointly with his counterpart in DAE Dr. D. S. Shukla. It was published in the year 2023.

Dr. Garg breathed for the last time on August 30, 2026.

A young R.K. Garg with the associates of Project Firewood - a term associated with early Uranium production activities in India. In this very old photograph from the archives of BARC, present next to Dr. Garg is Mr. N. Srinivasan, who was later associated with the establishment of India's maiden Reprocessing Plant in Trombay.





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**Independence Day
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