Q4 2025

QUANTUM VIBES

Inside the minds

Mr. Roberto Mauro,
Pasqal

QUANTUM CHEMISTRY ON QUANTUM COMPUTER

Dr. Atanu Bhattacharya
GITAM University Visakhapatnam

SCI 2025 SUPER COMPUTING INDIA 2025

QUANTUM CHEMISTRY AMONG THE STARS

Molecular Spectroscopy and Astrochemical Reactions

Dr. Sangita Sen
Mr. Pratyush Bhattacharjya
IISER Kolkata

FROM THE EDITOR

As we close out 2025, Quantum Vibes brings together a compelling snapshot of how quantum science is steadily transitioning from foundational theory to impactful practice across laboratories, computing platforms, and national infrastructures.

This edition opens with a deep dive into Quantum Chemistry on Quantum Computers, where Dr. Atanu Bhattacharya (GITAM University) explores how quantum algorithms are reshaping our ability to model complex molecular systems. Extending this journey beyond the laboratory, Dr. Sangita Sen and Mr. Pratyush Bhattacharjya (IISER Kolkata) take us among the stars, examining molecular spectroscopy and astrochemical reactions that connect quantum chemistry with the origins of the universe.

In our Inside the Minds section, we turn our focus to Neutral Atom Quantum Computing, featuring an insightful conversation with Mr. Roberto Mauro from Pasqal. The discussion sheds light on the rapid progress, scalability prospects, and architectural strengths of neutral-atom platforms in the global quantum race.

We also look back at Supercomputing India 2025, reflecting on the growing convergence of HPC, AI, and Quantum Computing, and the importance of co-design and hybrid architectures in shaping future computational ecosystems.

Our Quantum Currents section captures key national milestones, including India's first indigenous Quantum Diamond Microscope, an indigenous high-precision diode laser for quantum technologies, and the landmark announcement by the Hon'ble Union Minister, Dr. Jitendra Singh on establishing four state-of-the-art Quantum Fabrication and Central Facilities at IIT Bombay, IISc Bengaluru, IIT Kanpur, and IIT Delhi significant steps toward strengthening India's quantum hardware and manufacturing capabilities.

As always, we round off the issue with a curated list of upcoming quantum events in 2026, highlights from recent quantum publications, and a fun Qrossword puzzle for our readers.

Thank you for being part of the Quantum Vibes community. As quantum technologies continue to mature, we hope this edition informs, inspires, and sparks new conversations across the quantum ecosystem.

Happy Reading !

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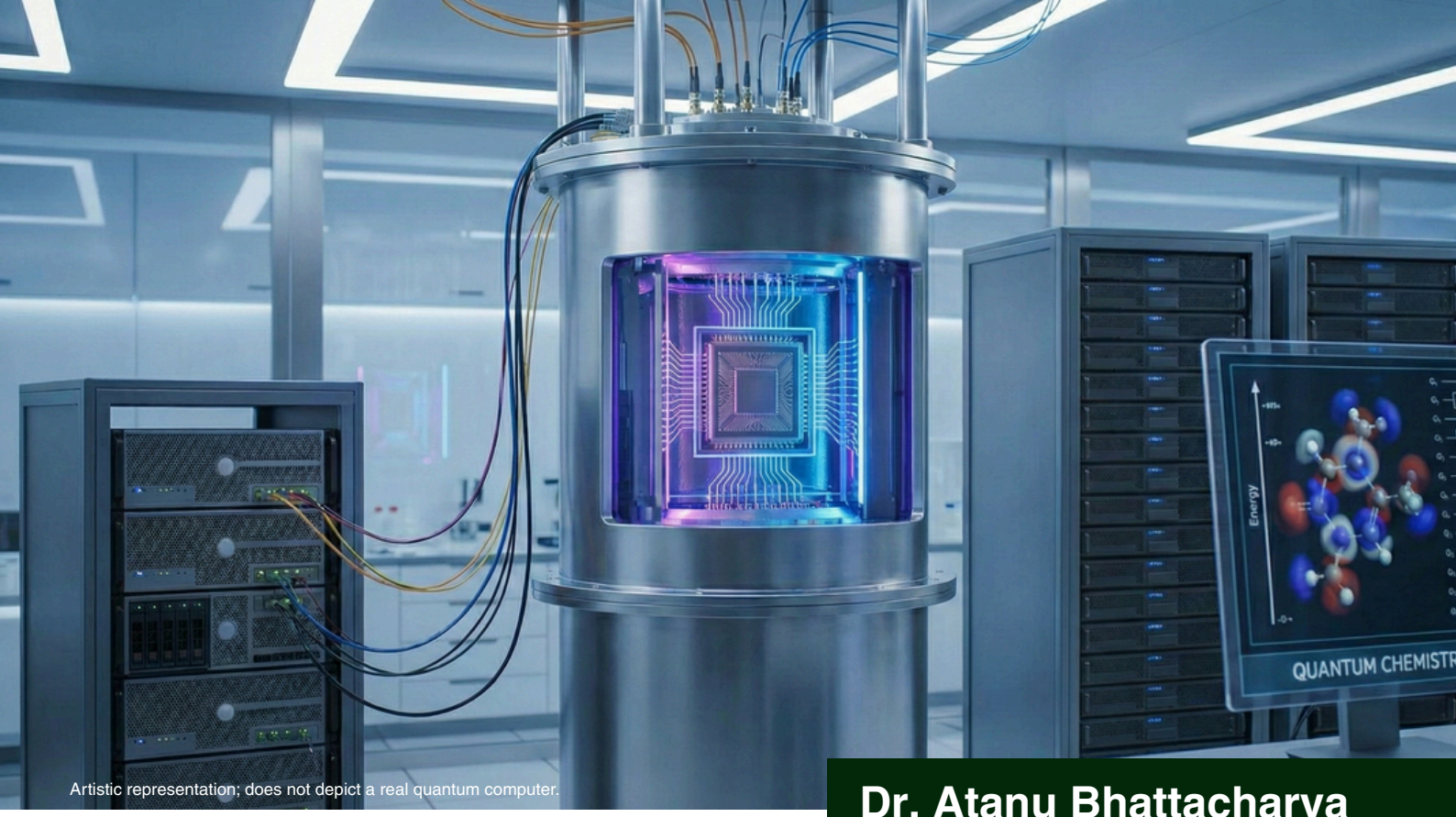


Artistic representation; does not depict a real quantum computer.

Dr. Atanu Bhattacharya

Quantum Chemistry on Quantum Computer

Quantum Chemistry and Computing: With the advancements in computer technology, it has become increasingly feasible to explain and predict chemical properties using quantum chemical calculations. These techniques are now widely applied across various branches of chemistry, including organic, inorganic, and physical chemistry. Computational quantum chemistry has played a significant role in several landmark scientific achievements[1]. For instance, the 1998 Nobel prize in chemistry recognized two major contributions to the field: Walter Kohn's development of density functional theory (DFT) and John Pople's creation of the Gaussian computational program. The following year, Ahmed Zewail was awarded the Nobel prize in chemistry for his pioneering work on ultrafast chemical dynamics, where computational quantum chemistry played a key role in interpreting experimental results[2]. More recently, the 2023 Nobel Prize in chemistry was awarded to Moungi G. Bawendi, Louis E. Brus, and Aleksey I. Ekimov for the discovery and synthesis of quantum dots – a field that extensively relies on quantum chemical computational methods for interpretation of the experimental results. Similarly, the 2023 Nobel Prize in physics was awarded to Pierre Agostini, Ferenc Krausz, and Anne L'Huillier for their contributions to attosecond science which also heavily depends on quantum chemical calculations[3]. These advancements have driven the development of numerous quantum chemistry software packages, both open-source and commercial, refined over decades. Notable examples are Gaussian, Gamess, Molpro, MCTDH, VASP packages. Today computational quantum chemistry is not only central to cutting-edge chemical research but also has become an indispensable component of modern chemical education[4,5].

Recent advancements in quantum computing algorithms and software have sparked significant interest in the potential of quantum computers for quantum chemical calculations[6,7]. There is growing curiosity among chemists, chemical engineers, material scientist, and professionals in chemical industry about its practical applications and relevance to the chemical sciences.

At first glance, quantum computing may appear to be just another computational tool for chemists. However, upon closure examination, it quickly reveals itself as a highly complex and non-intuitive field[8,9]. This complexity largely stems from its foundations in quantum mechanical concepts that are often not thoroughly covered in traditional chemistry or chemical engineering curricula and practices[9]. This leads a noticeable prevalence of misconceptions, often amplified by hype and jargon. Common examples include exaggerated claims such as: “Quantum Computing will revolutionize medicines, agriculture, drug discovery and material design”. Or “Quantum Computers will invent new catalysts to solve energy crisis”. While the aspirations are not entirely without merit, they frequently oversimplify the scientific and technical challenges involved.

One Illuminating Example

Consider the example of decomposition of energetic molecules following electronic excitations. Energetic materials are generally organic substances that store a large amount of chemical energy, which can be rapidly released through decomposition triggered by external stimuli (like a shock wave). They have numerous applications, including use as explosives, in pyrotechnic compositions, as high-energy propellants, and as fuels (some of which are illustrated in Figure 1).

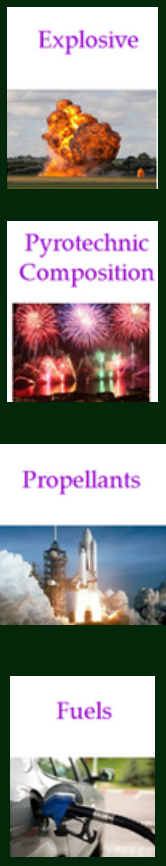


Figure 1: Different applications of the energetic materials.

The mechanism by which energetic materials release their stored chemical energy is an incredibly complex process. Energetic molecules universally release their stored chemical energy when subjected to typical initiation events. For instance, the application of shock waves or compression waves is a highly energetic process that can readily excite molecules to their electronically excited states. Figure 2, as an illustrative example, demonstrates how applying mechanical stress, shock, or pressure to solids often leads to the emission of luminescence, known as triboluminescence (TL) or mechanoluminescence (ML)[10]. These external stimuli excite energetic molecules to the electronically excited states, which is the crucial initial step in their energy release. Therefore, understanding the chemical dynamics of energetic molecules after electronic excitation is vital for a fundamental, molecular-level comprehension of their explosive and fuel properties.

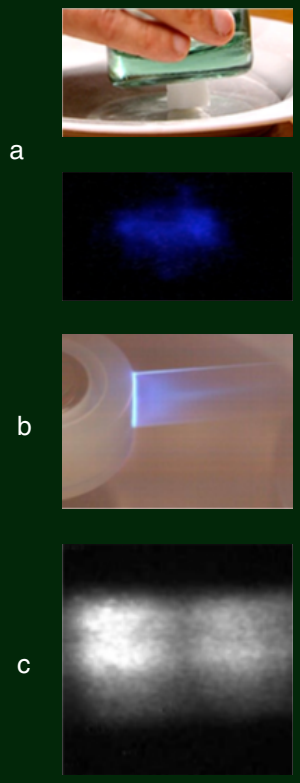


Figure 2: Observation of triboluminescence (emission of light due to pressure): (a) when a sugar cube is crushed with a flat-bottomed glass in darkness[11], (b) when the end of an ordinary adhesive tape is pulled away from the roll[12], and (c) when a diamond crystal is fractured due to pressure[13].

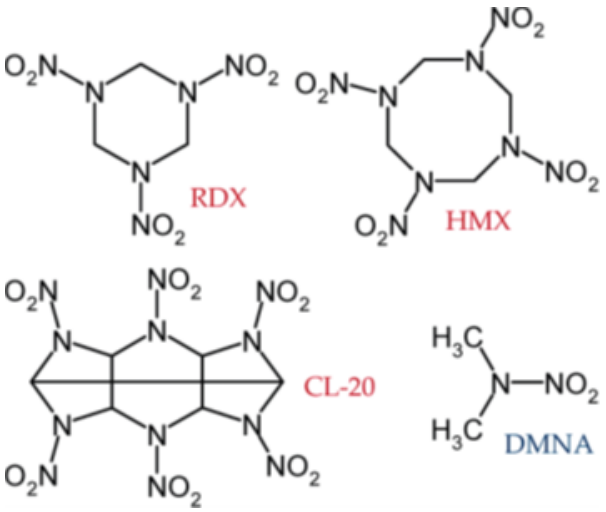


Figure 3: Chemical structures of RDX, HMX, CL-20, and dimethylnitramine (DMNA).

To date, several studies have investigated the decomposition mechanisms and dynamics of electronically excited energetic molecules particularly nitramine (-N-NO_2) compounds, such as RDX (1,3,5-trinitro-1,3,5-triazacyclohexane), HMX (1,3,5,7-tetranitro-1,3,5,7-tetraazacyclooctane) and CL-20 (2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane). The chemical structures of these molecules are shown in Figure 3. Upon electronic excitation, the RDX molecule undergoes dissociation, producing nitric oxide (NO) as a primary product[14]. The resulting NO exhibits a cold rotational distribution (~20 K) but a hot vibrational distributions (~1800 K), indicating that nitramine energetic molecules likely dissociate on the ground electronic state following rapid internal conversion from higher excited electronic states. This behavior is commonly attributed to the presence of a conical intersection that facilitates non-radiative relaxation and governs the decomposition pathway. A generic topography of potential energy curves with a conical intersection is presented in Figure 4. While this mechanism is well-established for small model systems (e.g., DMNA)[15], direct quantum chemical evidence supporting the role of conical intersections in the decomposition of large energetic molecules (e.g., RDX, CL-20) is currently lacking. It will soon become evident that this problem is unlikely to be solved using classical computers alone. A quantum computer is required to accurately explore the chemical dynamics of large molecular systems following electronic excitation.

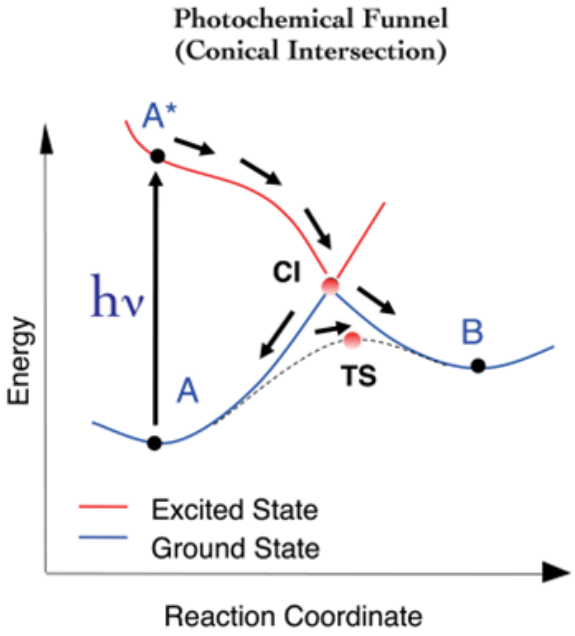


*Figure 4: A generic picture of conical intersection between two potential energy surfaces. In this figure, **CI** refers to the conical intersection and **TS** refers to the transition state. This figure is reproduced from I. Schapiro, F. Melaccio, E. N. Laricheva and M. Olivucci, Photochem. Photobiol. Sci. 10, 867 (2011), with permission of The Royal Society of Chemistry (RSC) on behalf of the Centre National de la Recherche Scientifique (CNRS) and the RSC.*

Need of a Quantum Computer

Given the limitations of current classical computers, both experimentalists and theoreticians often turn to simplified model systems in hopes of uncovering the intrinsic properties of larger, more complex molecules. Following this strategy, dimethylnitramine (DMNA), which contains a single N-NO_2 moiety (see Figure 3) has been investigated as a model nitramine system[14,15]. Interestingly, nitric oxide (NO) also emerges as a major decomposition product when DMNA dissociates after electronic excitation. However, contrary to expectations, the internal energy distributions of the NO product is found to be rotationally hot (120 K) but vibrationally cold, distinctly different from what is observed in RDX. This suggests that DMNA does not effectively replicate the decomposition dynamics of large nitramines, such as RDX, HMX, or CL-20. To truly understand the behavior of these complex energetic materials, direct studies on the molecules themselves are essential, as no simple model system appears to capture their key characteristics.

The above realization raises a critical question: how can we explore the quantum dynamics of RDX decomposition, particularly through its relevant conical intersections? As we will see, current classical computers are fundamentally limited in their ability to model such processes with full quantum mechanical details. So, how can quantum computers offer a solution? To answer this, we must first understand the foundations of molecular electronic structure theory calculations, as discussed in reference 16. For readers new to the field, a simplified overview is presented here. Every molecular electronic structure calculation begins with an initial guess for the total electronic wavefunction, parameterized in a specific way. These parameters are then iteratively optimized to minimize the system's energy with respect to the electronic Hamiltonian - a process known as the self-consistent field (SCF) method. The accuracy and predictive power of any such calculation ultimately depend on how well the electronic wavefunction is presented.

The Electronic Wavefunction

Consider a simple illustrative example: the lithium (Li) atom. Its ground-state electronic configuration is $(1s)^2(2s)^1$, but electronically excited states may involve configurations such as $(1s)^2(2p)^1$ or $(1s)^2(3s)^1$. Mathematically, each of these configurations corresponds to a distinct Slater determinant. Because electrons are indistinguishable and interact with one another, the most accurate description of the electronic wavefunction is a linear combination of multiple such determinants – concept known as configuration interaction. For the ground states, if the energy separation from excited configurations is large, a dominant single configuration (e.g., $(1s)^2(2s)^1$ for Li) is often sufficient. This is referred to as a single-configuration approach (see Figure 5). However, in electronically excited states, where several configurations may lie close in energy, this approximation breaks down. In such cases, a multiconfiguration approach is required, in which, the electronic wavefunction is expressed as a weighted sum of multiple configurations (also illustrated in Figure 5).

A powerful method for this is the Complete Active Space Self-Consistent Field (CASSCF) approach. It begins by selecting a set of active orbitals chemically relevant orbitals that include both occupied and unoccupied states and then distributing a chosen number of active electrons among them. For instance, in a CASSCF(10e,7o) calculation on DMNA, 10 electrons are distributed among 14 spin-orbitals (i.e., 7 spatial orbitals), generating all possible configurations consistent with the Pauli exclusion principle. Remarkably, this results in 1,001 distinct electronic configurations (reference 16 discusses how to calculate these numbers), which are combined to construct an accurate total electronic wavefunction that captures DMNA's excited-state behaviour. Such a dynamics simulation using a (10e,7o) active space – has been feasible with classical computers for relatively small molecules like DMNA[15].

Now, if we scale this same active space to RDX, which has three N-NO_2 units compared to DMNA's one, the number of required electronic configurations increases dramatically, reaching approximately 10^{10}. That's nearly 10^7 times more than that of DMNA case. This exponential growth in configuration space presents a major computational challenge.

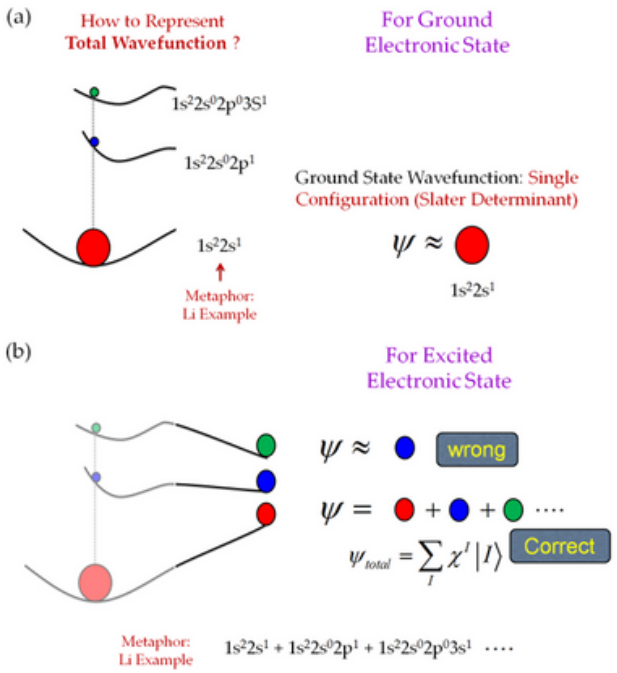


Figure 5: Representing lithium's electronic wavefunctions: ground vs. excited states; using a metaphorical example of a lithium atom, let's illustrate the appropriate representation of its total electronic wavefunction for: (a) the ground electronic state and (b) an excited electronic state.

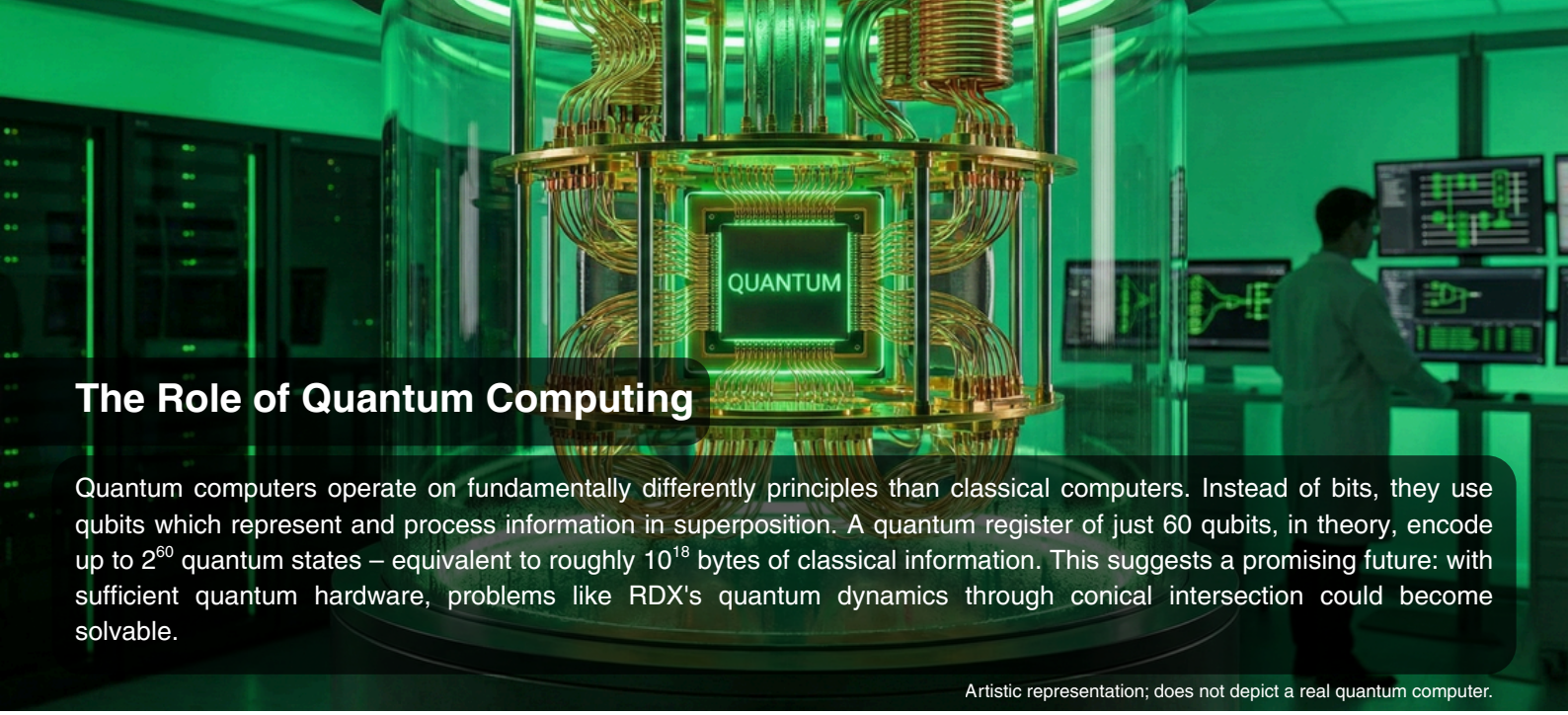
Suppose that handling DMNA's 1001 electronic configurations requires around 1 GB of memory. As memory requirements scale with the number of configurations often following a power-law-relationship we can estimate the memory needed for RDX using a simplified model. Apply the most basic power-law scaling, $\text{Memory} \propto (\text{Configuration})^2$, the memory required for RDX's 11058116888 electronic configurations would be approximately 10^{17} bytes. In stark contrast, even the most advanced classical supercomputers today offer memory capacities below 10^{15} bytes. And this challenge worsens when performing quantum dynamics simulations, where memory and computational demands grow even more steeply. This back-of-the-envelope estimate clearly illustrates the core issue: the RDX problem is not classically computable.

Myths

Quantum computers are chemistry superheroes that instantly solve any molecular puzzle.

Facts

In reality, they're more like curious interns still learning, capable of tinkering with tiny molecules in labs, and best when teamed up with classical computers and human chemists.



The Role of Quantum Computing

Quantum computers operate on fundamentally differently principles than classical computers. Instead of bits, they use qubits which represent and process information in superposition. A quantum register of just 60 qubits, in theory, encode up to 2^{60} quantum states – equivalent to roughly 10^{18} bytes of classical information. This suggests a promising future: with sufficient quantum hardware, problems like RDX's quantum dynamics through conical intersection could become solvable.

Artistic representation; does not depict a real quantum computer.

Chemical Systems beyond Energetic Materials

Numerous other chemically significant systems also require the capabilities of quantum computing, particularly in areas where classical computing falls short. This is especially true in fields such as EUV photolithography and any domain involving the photochemistry or electronic excitation /ionization of large molecular systems. One notable example is photopharmacology[17], an emerging multidisciplinary field at the intersection of photochemistry and pharmacology. It harnesses the unique ability of light to modulate the pharmacokinetics and pharmacodynamics of bioactive molecules, with the aim of precisely regulating drug activity in vivo through controlled light exposure.

In our lab, we are developing spatially and temporally controlled drug delivery systems, using light-cleavable "caged drugs" to achieve precise activation at diseased sites. Specifically, we synthesize conjugates of therapeutic molecules with the well-known dye BODIPY, an example of which is shown in Figure 6(a), and investigate their photochemical behavior using NMR and mass spectrometry.

Upon photoexcitation, multiple photochemical pathways can be activated in the BODIPY-drug conjugate. However, only one path that leads to efficient drug release is desirable. Identifying the molecular modifications needed to selectively enhance this productive channel remains a significant challenge.

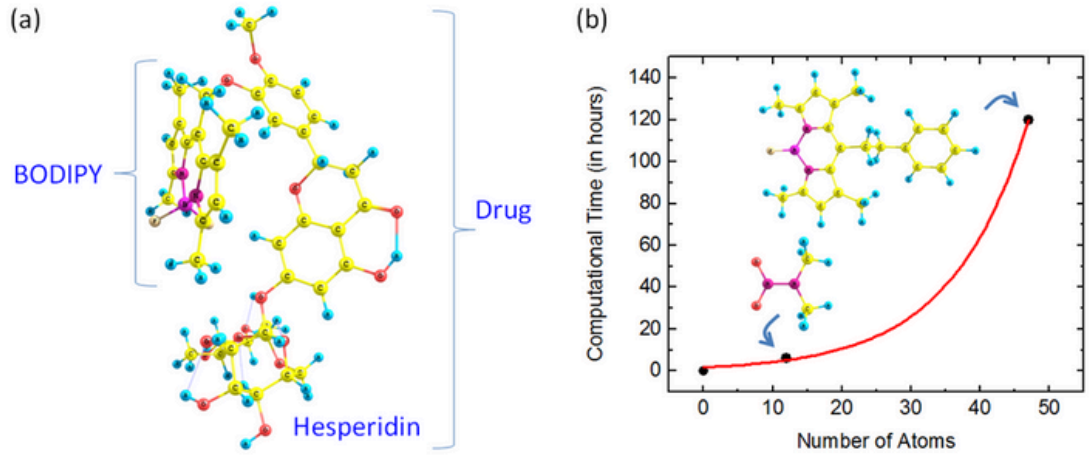
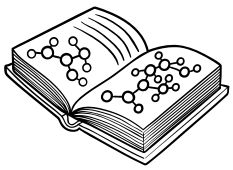


Figure 6: (a) Hesperidin, a natural anticancer phytochemical, is conjugated to the well-known dye BODIPY which absorbs visible light and enables the light-triggered release of Hesperidin. Due to the large size and complexity of this system, classical computers are currently unable to accurately model its photochemical dynamics. (b) A high-performance workstation - equipped with a 32-core CPU and 512 GB of RAM – requires approximately 1 hour to simulate 60 femtosecond (fs) of electronically excited state dynamics for the DMNA molecule using the CASSCF(8,6)/6-31G(d) level of theory on the S_1 excited state. In contrast, performing the same 60 fs simulation for the large BODIPY-Phenol conjugate (a model system of BODIPY- Hesperidin) at the CASSCF(6,5)/6-31G(d) level of theory takes approximately 5 days. This stark difference highlights the rapid escalation in computational cost with increasing molecular size and complexity. These benchmarks were obtained using the ab initio multiple spawning method as implemented in Molpro in our lab.

Quantum dynamics simulations could offer predictive insight into these reaction pathways. However, simulating electronically excited-state dynamics of large macromolecular systems is beyond the reach of classical computing. Even with a high-performance workstation the computational cost is prohibitive, as illustrated in Figure 6(b) for a model BODIPY-Phenol conjugate. A high-performance workstation equipped with a 32-core CPU and 512 GB of RAM requires approximately 5 days to simulate 60 femtosecond (fs) of electronically excited state dynamics for the model BODIPY-Phenol conjugate at the CASSCF(6,5)/6-31G(d) level of theory. To obtain a reliable estimate of bond dissociation pathway and population transfer between electronic states, a trajectory length of at least 500 fs is necessary. Moreover, statistical significance demands the comparison of 1000 such trajectories. A straightforward calculation based on these parameters reveals that completing this full set of simulations would take over 100 years on a single workstation! Although GPUs offer some performance acceleration over CPUs, they are still inadequate for performing full quantum dynamics simulations on systems of this complexity and size[18].

Approaches such as mixed quantum-classical dynamics, including ONIOM-like partitioning schemes that treat the small active site quantum mechanically and the remainder classically, have been proposed in literature[19]. However, these methods become unreliable when extensive electronic conjugation is present, as the boundary between the quantum and classical regions becomes difficult to define without loss of accuracy. Ultimately, the unique capabilities of quantum computing are essential to enable accurate and tractable simulations of photochemical dynamics in macromolecules without compromising on physical fidelity.



Quantum Dynamics

The dynamics of a quantum system can be explored by solving the time-dependent Schrödinger equation. This process begins with an initial quantum state and tracks the evolution of the wavefunction at a later time using:

$$\psi(x,t) = \hat{U}(t)\,\psi(x,0) = e^{-\frac{i}{\hbar}\hat{H}t}\,\psi(x,0)$$

where, $\hat{U}(t) = e^{-\frac{i}{\hbar}\hat{H}t}$ is the time-evolution operator, providing the formal solution for systems with a time-independent Hamiltonian[20].

Numerical implementation of the time-evolution operator can be performed through various methods. A widely used technique is the split-operator method, which approximates time-evolution over a small time step. As detailed in our earlier publications[20], the time-evolution operator is expressed in a symmetrised product form:

$$e^{-\frac{i(\hat{T}+\hat{V})\Delta t}{\hbar}} \approx e^{-\frac{i\hat{T}\Delta t}{2\hbar}}\, e^{-\frac{i\hat{V}\Delta t}{\hbar}}\, e^{-\frac{i\hat{T}\Delta t}{2\hbar}}$$

where, $\hat{T}$ and $\hat{V}$ denote the kinetic and the potential energy components of the Hamiltonian, respectively. In the position space, the kinetic energy operator corresponds to a non-diagonal matrix, making the direct computation of its exponential nontrivial. In contrast, diagonal matrices can be exponentiated element-wise. Since the kinetic energy operator becomes diagonal in momentum space, Fourier transforms are employed to switch between representations during numerical propagation.

In the context of quantum computing, these concepts naturally lead to use of the Quantum Fourier Transform (QFT) a fundamental algorithm in quantum computation. Our recent work explores these connections extensively, offering both pedagogical insights and broader applications[8,21]. The Crank-Nicholson method is another established approach for numerical propagation of quantum states. We are currently investigating whether the Crank-Nicholson scheme can be implemented using the HHL quantum algorithm.

In addition to the Hamiltonian, the initial wavefunction must also be mapped onto a quantum computing framework, a process known as initialization. We are currently exploring the initialization of wavepackets, a crucial step for simulating quantum dynamics on quantum hardware. The versatility of wavepacket methods is well established, with successful applications across a broad spectrum of chemical problems, including the calculations electronically excited state chemistry[15]. With our earlier humble expertise in wavepacket dynamics in classical computer, we focus on developing quantum algorithms tailored for macromolecular photochemical dynamics. In this context, several approaches to molecular dynamics through quantum computing frameworks are discussed in reference 22, which are also highly relevant.

Outlook and the Conclusions

The above discussion may give the impression that classical algorithms can be readily adopted for quantum computing. This adaption known as mapping the problem onto a quantum computing framework is a crucial step in quantum algorithm development. Several textbooks showcase numerous examples of quantum algorithms[23]. However, it may come as a surprise that many textbook quantum algorithms are not directly executable on today's real quantum hardware. This is primarily due to significant physical limitations, such as high error rates, limited qubit counts, short coherence times, and the environmental noise.

So, what we can do realistically at this stage? Chemistry readers new to quantum computing often encounter a widely discussed textbook algorithm called the Variational Quantum Eigensolver (VQE), which is frequently proposed as a tool for solving chemical problems such as those relevant to catalysis or agriculture. But is it truly practical and effective approach to use VQE for realistic chemical simulation at this point?

Let us momentarily shift our focus before returning to the above posed questions. It is worth reflecting on the tradition of computational chemistry in India. At present and to the best of our knowledge, India does not have a single homegrown software package for quantum chemical calculations. This is a sobering realization[24]. Have we truly cultivated a tradition of developing our own algorithms to solve chemically meaningful problems? Or have we primarily relied on software (free or commercial) developed abroad in an effort to compete in the global race of computational science?

I do not wish to answer these questions outright. Rather I invite readers, especially students, to reflect and investigate these issues themselves. They are deeply connected to how we engage with emerging fields like quantum computing with chemical application in mind. If a computational chemist aims to leap into quantum simulation by using today's quantum algorithms, such as those available via well developed platforms like Qiskit from IBM, and expects the same success as with classical packages like Gaussian, Molpro, MCTDH, or VASP, disappointment is likely inevitable. The field is still in infancy and current quantum hardware and algorithms are far from matching the robustness of classical computing infrastructures.

The Variational Quantum Eigensolver (VQE) was a landmark development – credited to Aspuru-Guzik and his team but it suffers from practical limitations. Extensions like ADAPT-VQE have attempted to overcome some of these challenges. More recently, sample-based quantum diagonalization has emerged as promising direction, showing that the field continues to evolve and refine its approaches[25].

This continual evolution is also reflected in the Gartner Hype Cycle[26], often used by investors and policymakers to assess technological readiness. As shown in Figure 7, quantum computing was predicted to become a mainstream application; however, this prediction did not materialize over time. According to such assessments, the quantum computing market is still fragile and in need of considerable time and development before it can deliver its full potential of quantum-acceleration in computational chemistry.

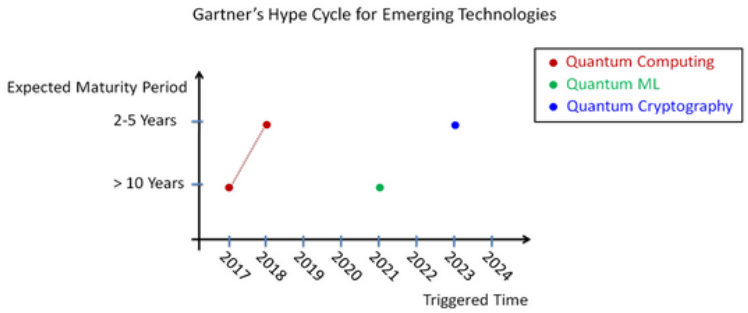


Figure 7: The intermittent emergence and disappearance of quantum technology in trend forecast makes it challenging to predict when this potentially transformative technology will mature. This figure was created using data from the Gartner Hype Cycle for the specified years.

In the end, there is a strong reason for optimism. While we may have missed the opportunity to build a strong tradition of developing our own chemical software in the classical computing era, the current momentum surrounding quantum computing offers a second chance. This emerging field provides us a rare opportunity to actively engage in algorithms development tailored for chemical applications from the scratch. History does not offer such chances often. It is up to us to recognize this moment and shape it with purpose.

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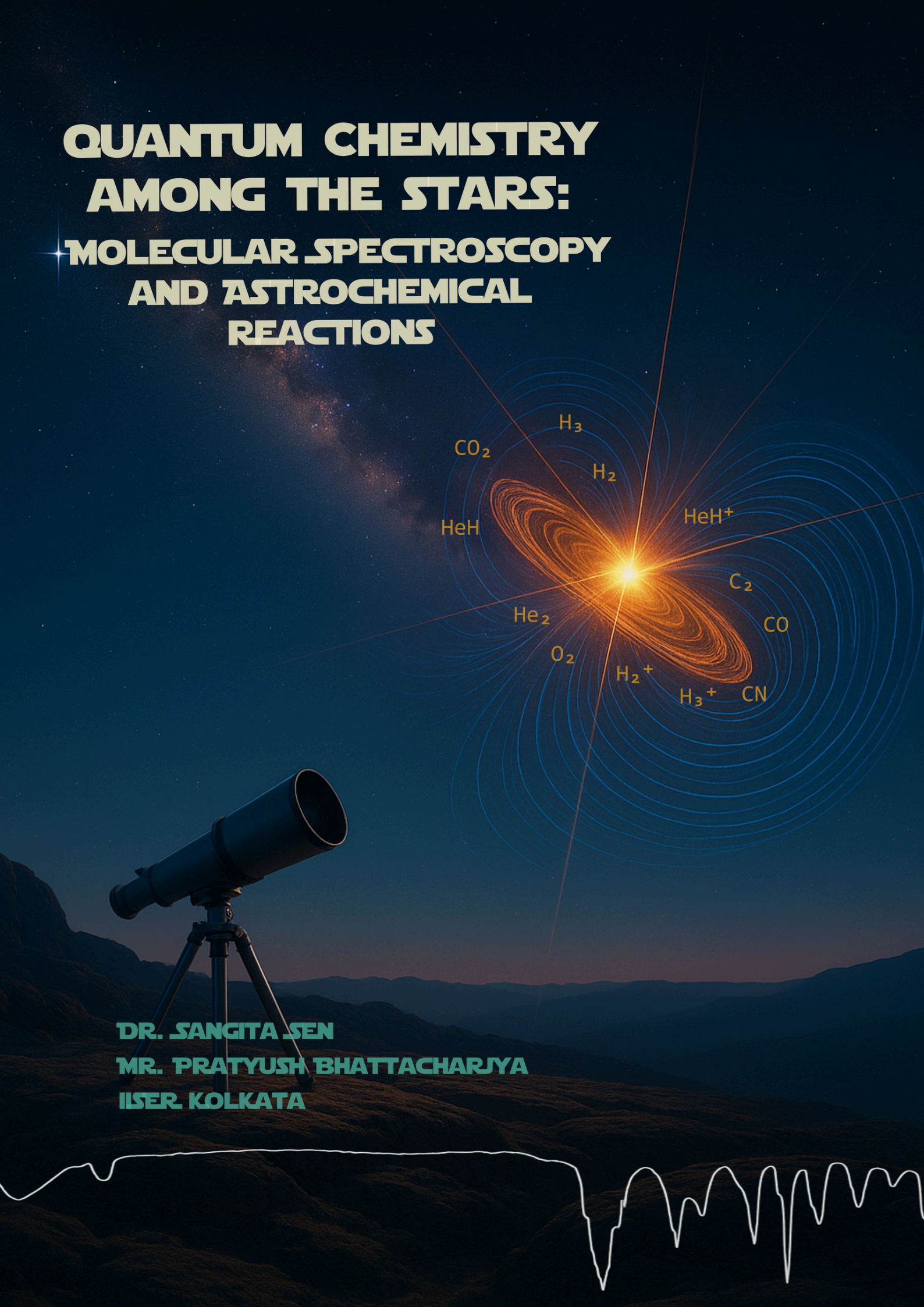
QUANTUM CHEMISTRY AMONG THE STARS:

MOLECULAR SPECTROSCOPY AND ASTROCHEMICAL REACTIONS



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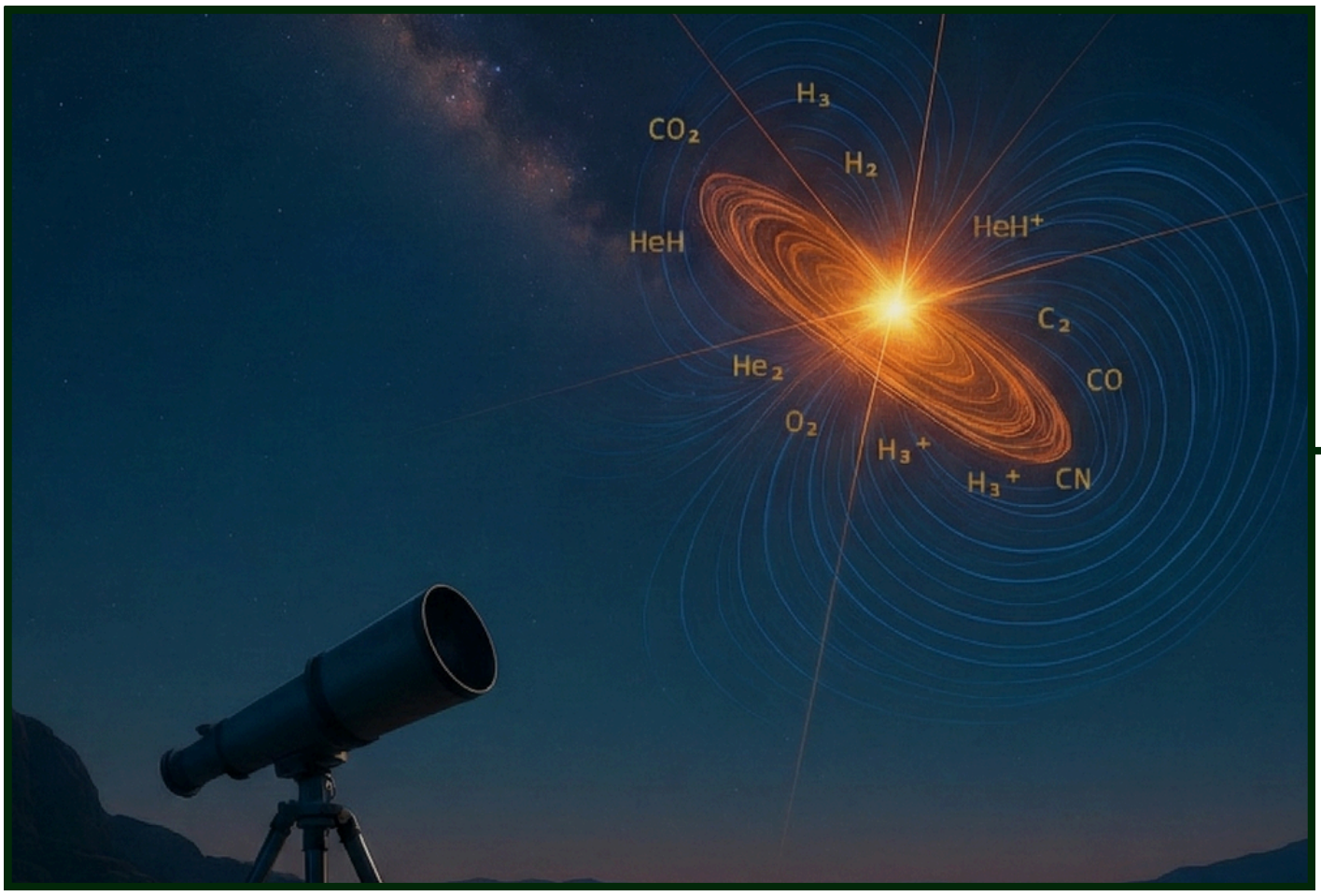
MR. PRATYUSH BHATTACHARJYA
IISER KOLKATA



Quantum Chemistry among the Stars: Molecular Spectroscopy and Astrochemical Reactions

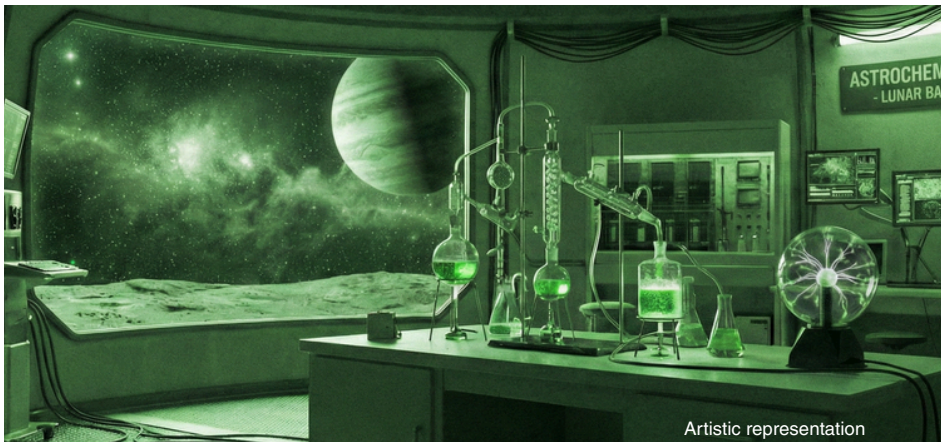
Dr. Sangita Sen
Mr. Pratyush Bhattacharjya
IISER Kolkata

Introduction

When we look up at the night sky, the twinkling dots of light often feel distant and immutable. Yet, between those stars, in the dark stretches of interstellar space, astonishing chemistry unfolds. The vast emptiness is not truly empty; it is filled with tenuous gases, icy dust grains, high-energy radiation, and magnetic fields, all conspiring to create a cosmic laboratory unlike any on Earth. The emerging field of **astrochemistry** seeks to understand these processes, i.e., how molecules form and evolve in space, how they interact with radiation, and how such chemistry may have seeded the origins of life. Despite the remoteness of these environments, we are not actually blind to them. Through the lens of spectroscopy, i.e. the science of analyzing light - astronomers can decipher the fingerprints of atoms and molecules across the Universe. Each molecule vibrates, rotates, absorbs, and emits radiation in unique ways, producing identifiable spectral lines. From these spectral signatures and clues, we piece together the puzzles that build up the frontiers of interstellar chemistry. Astrochemistry is a lot more than just cataloguing molecules.

It asks profound questions like: How do complex organic molecules arise in such harsh conditions? How do strong magnetic fields alter the rules of bonding and reactivity? Can our most advanced theories of electronic structure and dynamics i.e., tools designed in earthly computers and laboratories - capture the strangeness of the cosmos? And, looking ahead, could emerging frontiers like **machine learning** and **quantum computing** become the key to simulating such reactions? This article explores these questions, weaving together discoveries from spectroscopy, advances in theoretical chemistry, and the promise of quantum technologies.

The Cosmic Laboratory: Chemistry Among the Stars



Artistic representation

The space between stars, known as the interstellar medium, is almost unfathomably sparse: it contains on an average just a single atom per cubic centimeter. Yet, over millions of years, even these rare collisions can produce surprising complexity. Early astronomers assumed space contained only hydrogen and helium, but modern spectroscopy has revealed molecules such as carbon monoxide, ammonia, formaldehyde, methanol, and even simple amino acids drifting through interstellar clouds. The low density and frigid temperatures mean collisions are rare, so reactions often rely on processes that are inefficient in laboratories but powerful over astronomical timescales.

Charged molecules, such as H_3^+, react readily with neutral species even at near absolute zero. Sometimes, molecules stick together and release energy as light, a process known as radiative association. Tiny dust grains, coated with ice, serve as miniature laboratories where hydrogen atoms can combine into H_2, and more complex organic molecules can form. Even deep within clouds, high-energy photons and cosmic rays break molecular bonds, triggering new chemistry. These pathways together create the rich molecular diversity of the interstellar medium.

Different regions of space host distinct chemistry. In diffuse clouds, ultraviolet light triggers reactions among partially ionized gases. Dense molecular clouds, cold and dark, provide icy dust grains where atoms and molecules can meet and react. Around dying stars, circumstellar envelopes forge new molecules in stellar winds. And in star-forming regions, turbulent clouds produce new stars and planets, with heat and shocks driving further chemistry. Each environment offers unique conditions - temperature, density, and radiation - that shape the chemical pathways available.

Apart from temperature, density and radiation, magnetism could play a critical role in deciding the chemical phenomena occurring in space. Magnetic stellar objects like magnetic white dwarfs and neutron stars represent the most intriguing and extreme manifestations of magnetism in the universe. These confined remnants of stellar evolutionary fate possess magnetic fields which are a billion times stronger than those found on Earth.

Under the cosmic weight and fierce magnetism of these objects, matter seems to rewrite its own laws - atoms stretch, bonds transform, and our terrestrial language of chemistry finds no words to describe such order and chaos. Chemistry itself becomes something alien! We'll be talking more about it as we move along.

Spectroscopy: Light as a Cosmic Forensic Tool

Spectroscopy remains the cornerstone of our understanding of extraterrestrial chemistry. Every discovery of a new molecule in space, be it water vapor in protoplanetary disks or methanol in star-forming clouds owes its existence to precise spectral analysis. Modern radio telescopes like ALMA (Atacama Large Millimeter/submillimeter Array) and infrared observatories like **JWST (James Webb Space Telescope)** are extending this reach, detecting faint rotational and vibrational lines from complex molecules even in distant galaxies.

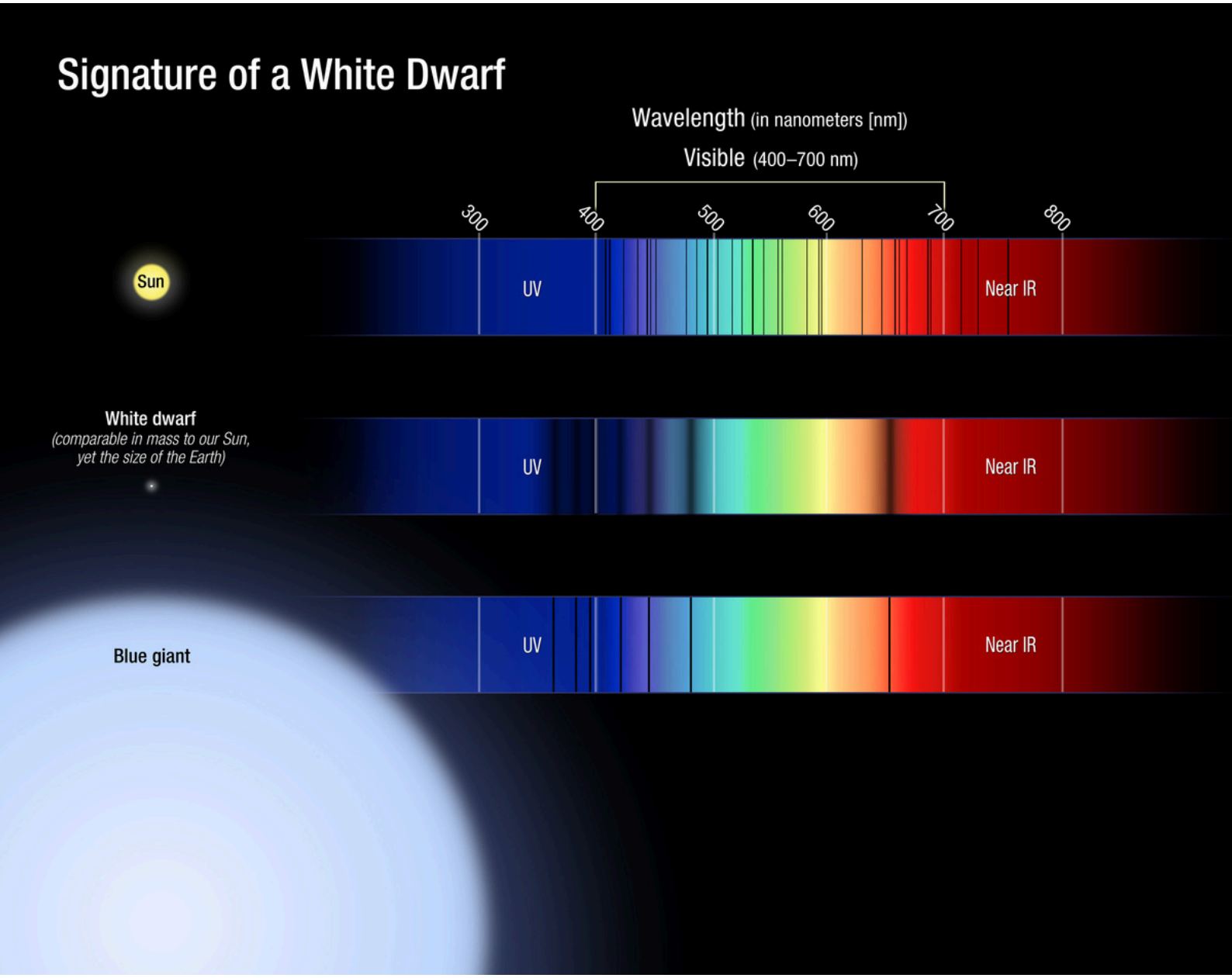


Figure 1: The broad, deep hydrogen absorption lines in a white dwarf's simple spectrum - caused by intense surface pressure - allow astronomers to accurately determine its mass and temperature. (Image courtesy: NASA)

Spectral patterns (like in Figure 1) provide not only chemical identities but also physical and dynamical information - such as temperature, density, and motion of the observed regions. For example, line broadening reveals turbulence or rotation, while intensity ratios offer clues about excitation mechanisms. Laboratory astrochemistry and quantum simulations play a vital role here, ensuring that the spectra interpreted from space correspond accurately to real molecular transitions. Without quantum-level insight into these spectra - especially radicals, ions, and excited states - the molecular inventory of the cosmos would remain incomplete.

Electronic Structure and Nuclear Dynamics: The Quantum Framework

At the heart of astrochemistry lies the interaction between electrons and nuclei under extreme conditions. Predicting the spectra, reaction rates, tunneling probabilities, or molecular stability in such environments requires a seamless blend of **electronic structure theory** and **quantum nuclear dynamics**.

Electronic structure methods - **Density Based Methods (DFT)** and **Wavefunction based methods (CASSCF, MRCI, MRCC, CCSD(T),** etc) - help define Potential Energy Surfaces (PES) that describe how electronic energy changes as nuclei move (under the Born Oppenheimer Approximation). In our group we leverage our in-house Multireference theories like **UGA-SSMRPT2**[1] and the Coupled Cluster variants[2], to construct accurate PESs. For example, Figure 2 presents the interaction potential energy surfaces for a hydrogen atom approaching an H_2 molecule along different angular orientations with respect to the H-H bond, obtained from UGA-SSMRPT2 calculations. This wavefunction based theory just like any other of its kind, must follow size-extensivity and consistency criteria to be useful in PES constructions. Additionally, they must be computationally feasible as tens of thousands of single-point calculations must be performed by scanning the interesting parts of the internuclear distance space, even for a system involving three atoms. On these PESs, the nuclei dance according to quantum mechanics - sometimes classically along smooth valleys, sometimes tunneling through barriers that seem impassable.

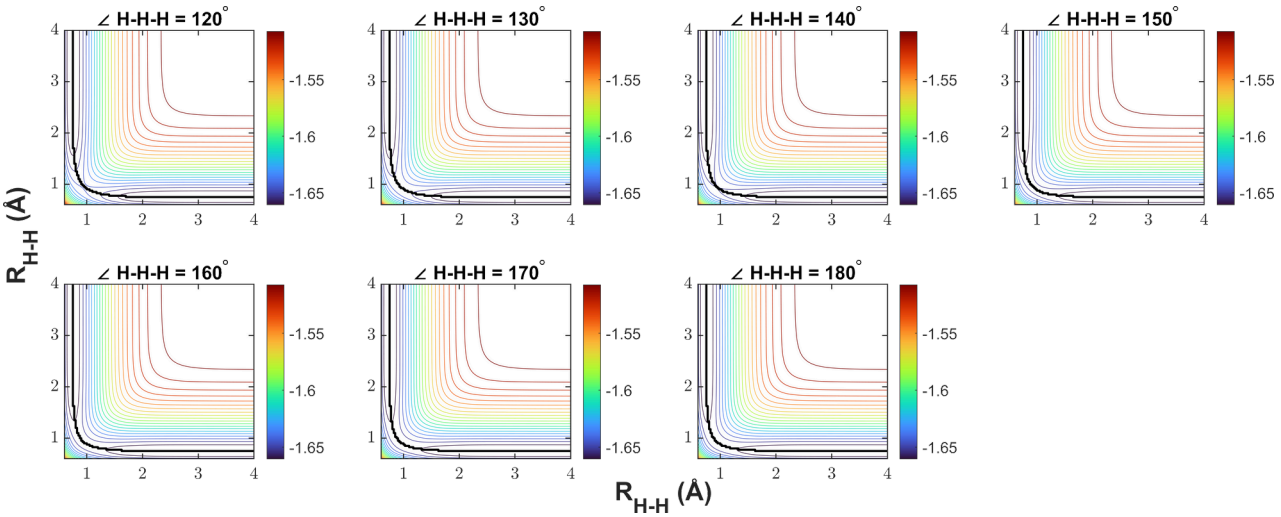


Figure 2: A 2D visual representation of the PES computed for the reaction, $H + H_2 \rightarrow H_2 + H$, using UGA-SSMRPT2 at various internal angles. The black line is representative of the minimum energy pathway of the reaction along that angular orientation.

To simulate these dances, one can use **wave packet propagation** techniques[3] of varying orders or **MCTDH (Multi-Configuration Time-Dependent Hartree)**[4] approaches, capable of describing how vibrations, rotations, and electronic states interact. In astrochemical contexts, these methods help unravel how molecules survive and react in ultra-cold clouds or near hot stars, and how simple atoms can be assembled into interesting molecules under such delicate quantum choreography. In our group, we develop and apply algorithms of Quantum Dynamics to solve the nuclear problem for reactive and non-reactive scattering problems to validate our electronic structure theories for earthly reactions thereby ensuring their ability to handle astrochemical environments. The computation of electronic and ro-vibrational spectra helps us uncover the spectral signatures of molecules under extreme conditions enabling their discovery in astrochemical environments. Our group currently works on simulating spectra in the presence of magnetic fields of the order of gigatesla which are currently impossible to generate in experimental laboratories.

Chemistry Under Strong Magnetic Fields

Magnetic fields pervade the cosmos - from gentle interstellar ones to the extreme mega- or giga-tesla fields near magnetized white dwarfs and neutron stars. In such regions, chemistry does not obey the familiar rules of terrestrial environments. Magnetic fields distort electronic orbitals, mix spin states, and reshape potential energy

surfaces[5] [6] [7], leading to unusual bonding patterns and reaction channels. We call them exotic conditions!

To accurately describe electronic energies of molecules in strong magnetic fields, it is essential to employ **gauge-including atomic orbitals (GIAOs)**, also known as London orbitals[8]. GIAOs incorporate the vector potential of the magnetic field directly into the atomic basis functions, ensuring that calculated properties such as energies, magnetic susceptibilities, and current densities are **gauge-origin invariant**. This is crucial because conventional electronic structure methods without gauge correction can produce unphysical results when external fields are present.

Using **GIAO-based methods implemented in software like LONDON**[9], we can perform **CCSD(T)** and **CASSCF** calculations that capture both electron correlation and the interaction of electrons with strong magnetic fields. It can be shown how magnetic fields deform electronic orbitals[5], induce current densities[10], and modify spin couplings, effects that conventional zero-field theories fail to capture.

On the nuclear front, we strive to solve the complicated nuclear dynamics problem in the presence of strong magnetic fields. In a recent work from our group, Yenugu et. al.[11] demonstrated the applicability of the gauge invariant Wilson Hamiltonian in solving the quantum nuclear Schrodinger equation in the presence of astrochemically strong magnetic fields. The single-particle Hamiltonian was adapted for two particles, yielding strong field rovibrational spectra of molecules like H_2 (Figure 3). The diagonalization scheme was studied in this work. Alongside that, the Imaginary Time Evolution Method (ITEM) was also employed, which uses a very clever trick of propagation to obtain eigen states and vectors.

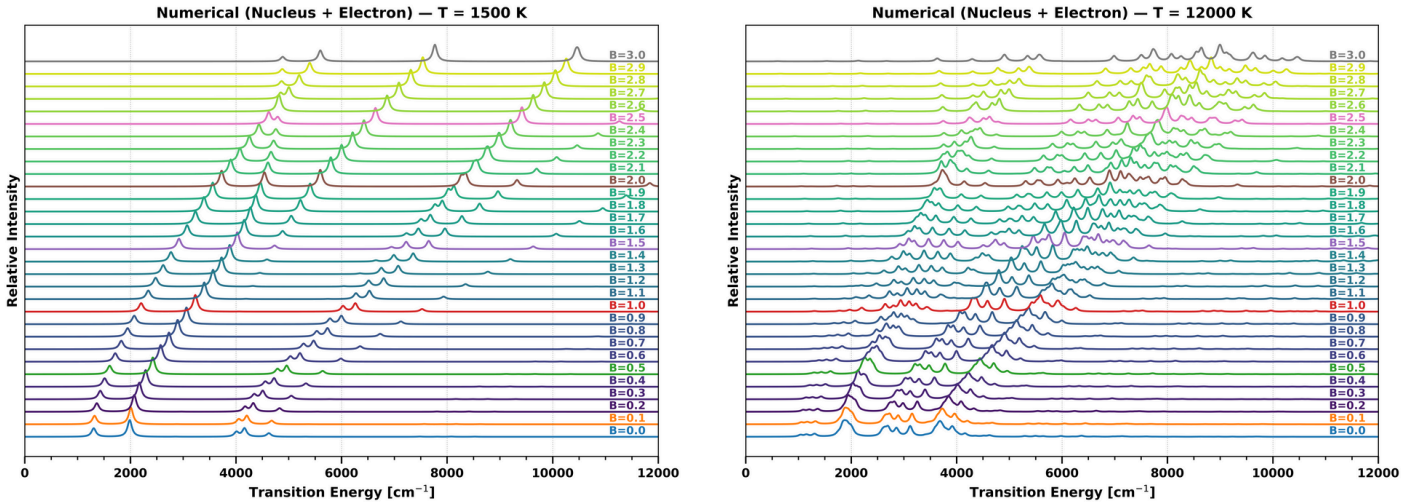


Figure 3: Simulation of IR-spectra of H_2 in the presence of strong magnetic fields of astronomical magnitudes in white dwarfs at surface temperatures of 1,500K (left) and 12,000K (right). The spectra are unrecognizable compared to the field free scenario and change dramatically on increasing the strength of the magnetic field.

We are working on expanding our horizons to understand real-time wavepacket propagation to solve the quantum dynamics problems involving high-dimensional Hilbert spaces and analyze a multitude of different higher-order propagator schemes, consequently discovering the most computationally efficient, accurate and stable scheme among them all.

Machine Learning and Quantum Computing: The New Frontier

The explosion of data - from astronomical spectra to quantum simulations - has positioned **machine learning (ML)** as a paradigm-shifting tool in astrochemistry. ML models can infer potential energy surfaces with near-quantum accuracy but at a fraction of the computational cost, enabling long-time dynamical simulations of large systems previously inaccessible to a varied set of ab initio methods. Neural networks and Gaussian Regression models are increasingly used to classify unknown spectral lines, predict molecular abundances, and explore reactive pathways in vast chemical networks.

We have worked on fitting our Potential Energy Surfaces using highly accurate ML neural network methods like the

Permutation Invariant Polynomial Neural Networks (PIP-NNs)[12] using various activation functions for the purpose of Quantum Dynamics studies. We also work on solving the quantum dynamics problems mentioned above with **Physics-Informed Neural Networks**[13] and **DeepONets**[14], which provide mesh-free scalability and can tackle high-dimensional Hilbert spaces and parameter sweep in our problems of interest.

Quantum computing, on the other hand, represents another paradigm shift. Unlike classical computers, which approximate quantum systems, quantum devices simulate them directly. Techniques like the **Variational Quantum Eigensolver (VQE)**[15] and **Quantum Phase Estimation (QPE)**[16] promise exact solutions to electronic structure problems, particularly for systems with strong correlation and magnetically induced complexity.

When combined, ML and quantum computing form a synergistic loop: ML can guide quantum algorithms by predicting efficient ansatz or reducing search spaces, while quantum processors can provide training data for ML models based on first-principles accuracy. This hybrid approach holds the potential to revolutionize simulations of interstellar reactions - especially those involving magnetic effects, tunneling, and multi-state dynamics - marking a leap beyond the classical computational frontier.

Conclusions

Astrochemistry stands at an extraordinary crossroad, where observational, theoretical, and computational sciences converge. Spectroscopy gives us the eyes to detect molecules light-years away. Quantum chemical and dynamical methods explain how those molecules form and evolve under cosmic conditions. Strong magnetic fields challenge our understanding of electronic structure, forcing theory to adapt. And now, machine learning and quantum computing are transforming how we simulate and predict such phenomena.

In our group, we explore these frontiers through multireference electronic structure theories, quantum dynamics, and the study of molecular behavior in strong magnetic fields - linking fundamental quantum chemistry with astrochemical environments, with inclination towards the unexplored regimes where strong correlation, extreme fields, and quantum effects converge in novel ways and are, as of now, inaccessible to terrestrial experiments.

Together, these developments blur the boundary between chemistry and astrophysics. They remind us that the Universe is not only governed by stars and gravity, but also by the subtle choreography of electrons and nuclei - dancing the quantum tune of the cosmos. In decoding that music, we come closer not only to understanding the chemistry of the stars but also the origins of the molecules that make us.

Acknowledgements

We gratefully acknowledge the computational resources provided by **IISER Kolkata** and also **National Supercomputing Mission (NSM)** for providing computing resources of **'PARAM RUDRA'** at **S.N. Bose National Centre for Basic Sciences**, which is implemented by **C-DAC** and supported by the **Ministry of Electronics and Information Technology (MeitY)** and **Department of Science and Technology (DST), Government of India**.

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As a postdoctoral researcher at the Hylleraas Centre, University of Oslo, with Dr. Erik Tellgren, she investigated molecular properties and electronic excitations in strong magnetic fields. Her research group at IISER Kolkata focuses on molecular properties, excitations, and reaction dynamics in strong magnetic fields, as well as the development of quantum chemical methods for strongly correlated systems, electron correlation and spin adaptation, and emerging quantum computing applications. (*https://www.iiserkol.ac.in/~sangita.sen/*)

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Inside the minds

Exclusive Interview

Roberto Mauro

CEO, Asia Pacific

Pasqal's

Asia-Pacific business Lead

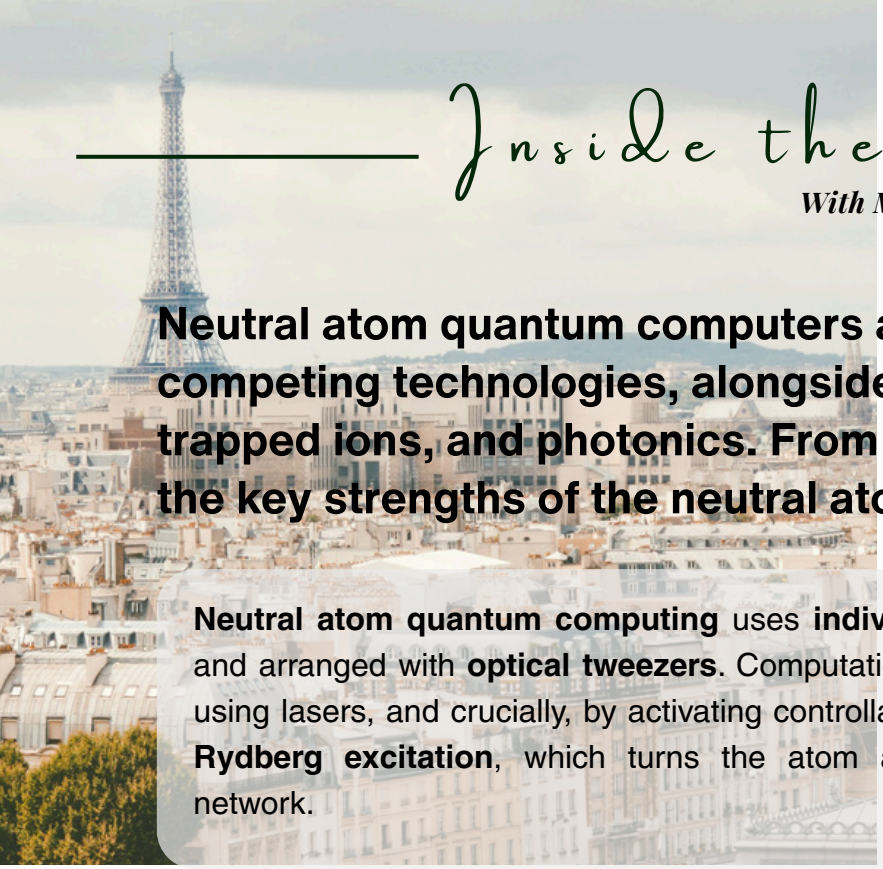
Building

STRATEGY INNOVATION & ECOSYSTEM

30 years of experience across quantum, AI, and digital technologies

LEADING

the way in Neutral Atom Quantum Computing



Inside the minds

With Mr. Roberto Mauro

Neutral atom quantum computers are one of several competing technologies, alongside superconducting qubits, trapped ions, and photonics. From your perspective, what are the key strengths of the neutral atom approach?

Neutral atom quantum computing uses **individual neutral atom as qubits**, trapped and arranged with **optical tweezers**. Computation comes from controlling atomic states using lasers, and crucially, by activating controllable interactions between atoms through **Rydberg excitation**, which turns the atom array into a programmable interaction network.

Key strengths and how this compares to other modalities:

1

Scalability

Neutral atom consists of **trapping atoms using optical tweezers**, then arranged as a **register**. Connectivity comes from laser-controlled Rydberg interactions, allowing **scaling capacity** that does not require additional complex interconnection. Pasqal's roadmap targets **10,000 qubit counts within a single QPU**, with **no technological obstacle to do so**, and without requiring multi-QPU interconnection as first scaling step.

2

Natural qubits

Atoms are **identical by physics**, which reduces device-to-device variability at the qubit level compared with other technologies (e.g., superconducting or silicon approaches), where uniformity is tightly linked to manufacturing dispersion.

3

Reconfigurable connectivity at scale

Neutral atom allows to position qubits in flexible 2D/3D geometries, so connectivity is **not locked by fixed configuration**. This is a structural advantage compared to those other technologies where layout and couplers are physically fixed, and routing constraints become central as systems grow.

4

Deployment-friendly

Neutral atom systems operate **without the millikelvin dilution refrigeration** required for other platforms, which simplifies infrastructure constraints for real deployments. This is a meaningful practical advantage when integrating into HPC/data-center environments.

5

Simulation and analog/digital-analog workflows

A strong fit for simulation and analog/digital-analog workflows: programmable interaction graphs make neutral atom particularly useful at **quantum simulation** and **analog / digital-analog** approaches where interaction structure is the core object, often more direct than approaches that rely on mapping everything into fixed gate layouts.

> **The neutral atom technology strengths demonstrate recent tangible milestones within the ecosystem: neutral atom platforms have demonstrated large-scale trapping (Pasqal reported arrays exceeding 1,000 atoms in optical tweezers), and the modality is being integrated within blue chip tech companies through partnerships (most notably Pasqal-IBM partnership).**

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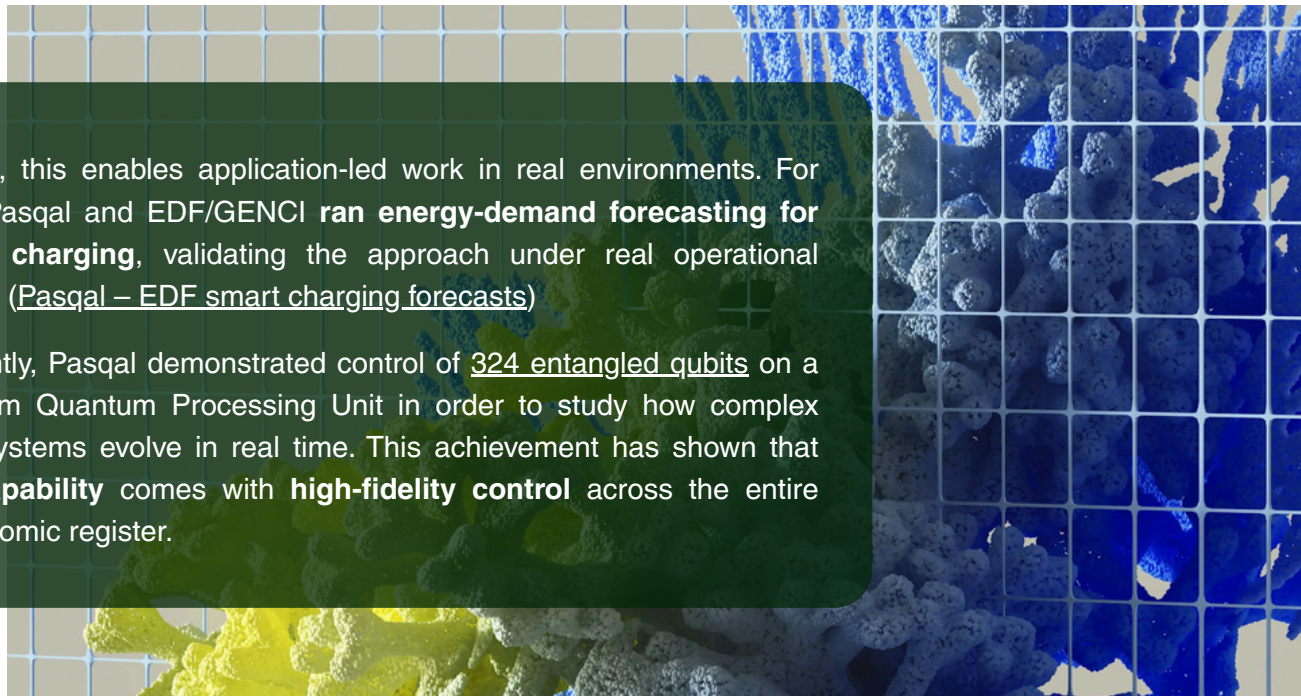
Pasqal's systems rely on optical tweezers and highly programmable atom arrays. How do these hardware choices translate into practical advantages for solving real-world problems such as combinatorial optimization or quantum simulation?

Optical tweezers allow Pasqal **shaping quantum registers to the use case**: atoms can be arranged in reconfigurable 2D/3D geometries, so the interaction graph is not constrained by fixed configurations. This is a direct advantage for **quantum simulation**, where interaction-driven Hamiltonian can be implemented naturally on programmable Rydberg arrays.

For **combinatorial optimization**, the same hardware flexibility translates into **more native encodings**: many real problems reduce to graphs (nodes/edges, constraints, penalties). With programmable arrays and interactions, Pasqal can encode these structures more directly than fixed-connectivity architectures.



Practically, this enables application-led work in real environments. For example, Pasqal and EDF/GENCI **ran energy-demand forecasting for EV smart charging**, validating the approach under real operational constraints. (Pasqal – EDF smart charging forecasts)

More recently, Pasqal demonstrated control of 324 entangled qubits on a neutral atom Quantum Processing Unit in order to study how complex quantum systems evolve in real time. This achievement has shown that **scaling capability** comes with **high-fidelity control** across the entire quantum atomic register.

Neutral atom systems are designed to plug into hybrid compute settings: Pasqal delivered a **Quantum Processing Unit to CEA (GENCI-TGCC) in France, and a second to Jülich Supercomputing Centre in Germany**, for integration with supercomputers, and was selected by EuroHPC for **EuroQCS-Italy at CINECA** (with a planned hybrid analog/digital upgrade), supporting iterative workflows from emulation/digital twins to hardware runs.

(Pasqal – GENCI & CEA delivery) (Pasqal–Jülich) (The Quantum Insider – EuroQCS-Italy)

Pasqal offers tools like Pulser and Pulser Studio for programming neutral atom devices. How do these tools help bridge the gap between low-level quantum control and application-level development, and who do you see as the primary users of this software stack?

From day 1, Pasqal was born as a **full stack integrated company**, developing **hardware, middleware, software** and **applications**, to **provide enterprise grade quantum solutions**.

Pulser provides a high-level Python interface to design, simulate, and execute pulse sequences on Pasqal's neutral atom Quantum Processing Units, exposing the physical capabilities of the hardware without requiring users to operate at laboratory control systems level. This **significantly reduces the gap between theoretical design and execution** on **real quantum hardware** – one of the near-term quantum experimentation principal bottlenecks.

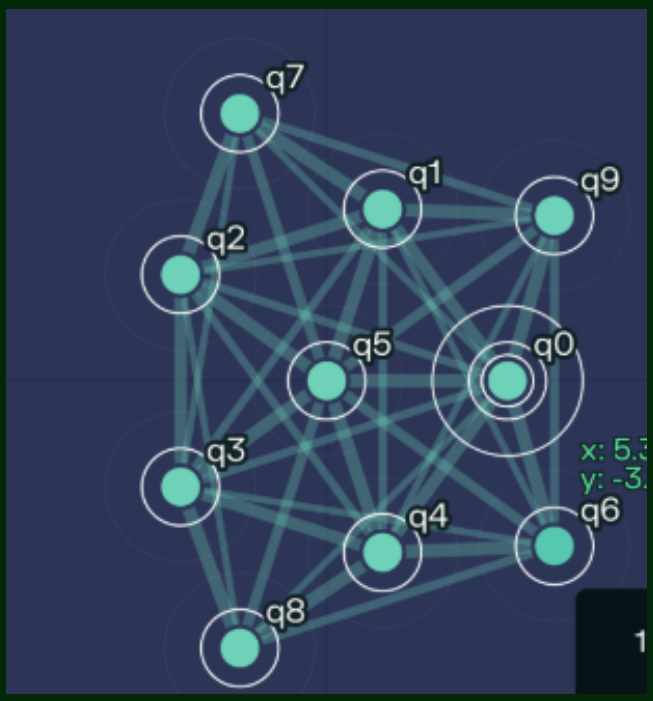
Pulser Studio complements this approach by offering a **visual, no-code environment** for rapid prototyping and onboarding.

All together, these tools primarily serve researchers and quantum engineers, industrial teams conducting structured proof-of-concept studies, and users building skills through education and training. By providing open-source tools like **Pulser** and cloud-based access to hardware, Pasqal **lowers the barrier for researchers, developers**, and **industrial teams to experiment, learn**, and **build expertise without heavy upfront investment**. This approach accelerates adoption by enabling a broader community to engage with the technology, validate ideas, and develop reusable workflows. It also supports transparency and reproducibility, which are essential for building trust and credibility.

In **addition to the programming tools**, Pasqal has also **developed ready to use libraries** like for example **QEK** (Quantum Evolution Kernel) that further accelerates adoption for enterprise users. (Pasqal–QEK)

Inside the minds

With Mr. Roberto Mauro



With Pasqal's cloud platform, what insights have you gained from how users actually interact with the hardware?

Pasqal Quantum Processing Units are accessible via **major cloud platforms** (Microsoft Azure Quantum, Google Cloud, OVHcloud, Scaleway) and through **Pasqal's native Cloud**. Pasqal provides access through the cloud to its QPUs installed **in Europe, in North America**, and **soon in Asia**. (Pasqal–Azure Quantum); (Pasqal–Google Cloud Marketplace); (Pasqal–OVHcloud Quantum Platform);(Pasqal–Scaleway); (Pasqal Cloud).

Cloud access has clarified three practical insights about how users interact with neutral atom hardware.

Sustained demand concentrates around structured environments.

The most visible recurring usage comes from **HPC, national infrastructures**, and **partners** running multi-month jobs rather than one-off run.

Usage is iterative and workflow-driven.

Teams typically prototype and debug pulse programs using **emulators**, then run on the QPU, compare outcomes, and iterate. This makes experimentation more reproducible and shortens the test and learn cycle.

Workloads are very background diversified.

Neutral atom systems are especially well suited to **quantum simulation** and **digital-analog experimentation**, and to application-led studies where partners test value under operational constraints.

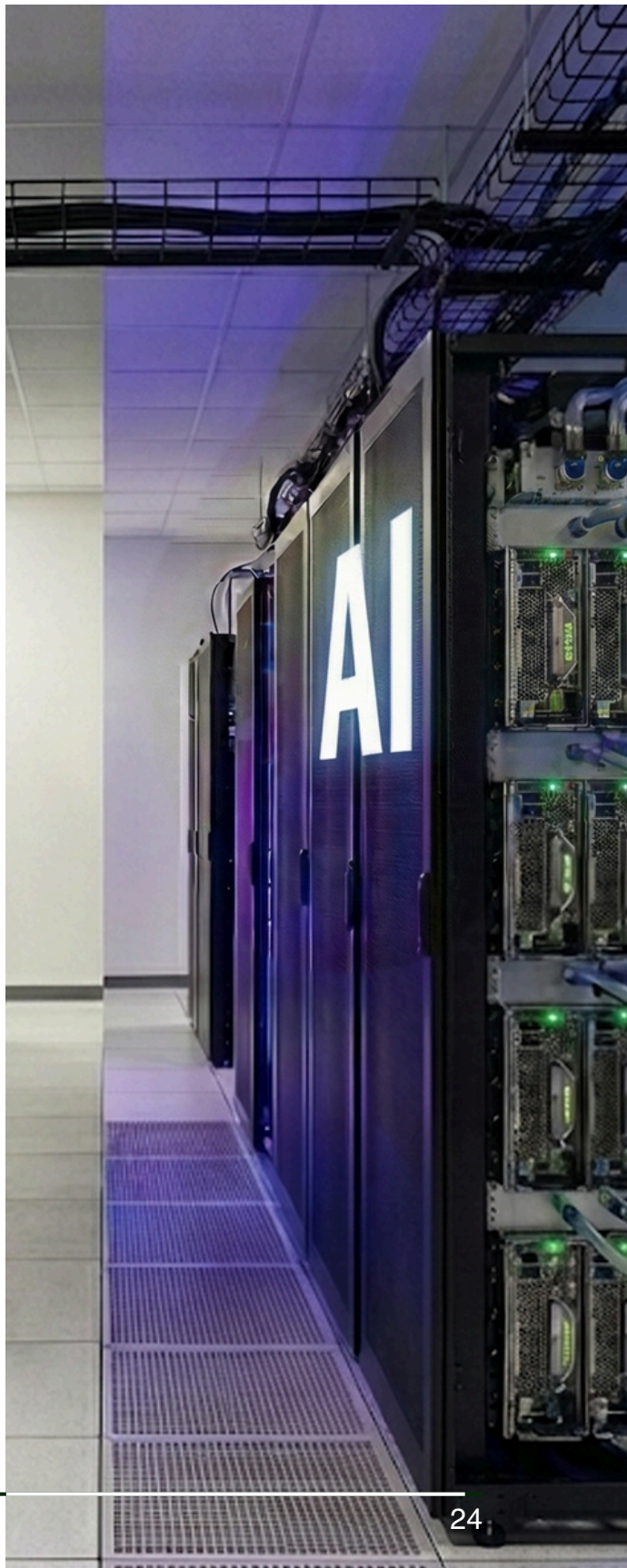
There is growing interest in hybrid architectures that integrate quantum processors with classical HPC and AI systems. How does Pasqal position its technology within such hybrid workflows, and what technical or architectural challenges still need to be addressed?

Pasqal seeks to **integrate its Quantum Processing Units within the HPC environment**, so the QPU can be invoked among others as a compute resource inside classical workflows. This is the direction of Pasqal-IBM **HPC-QC integration partnership**, focused on integration patterns for hybrid quantum-classical execution.

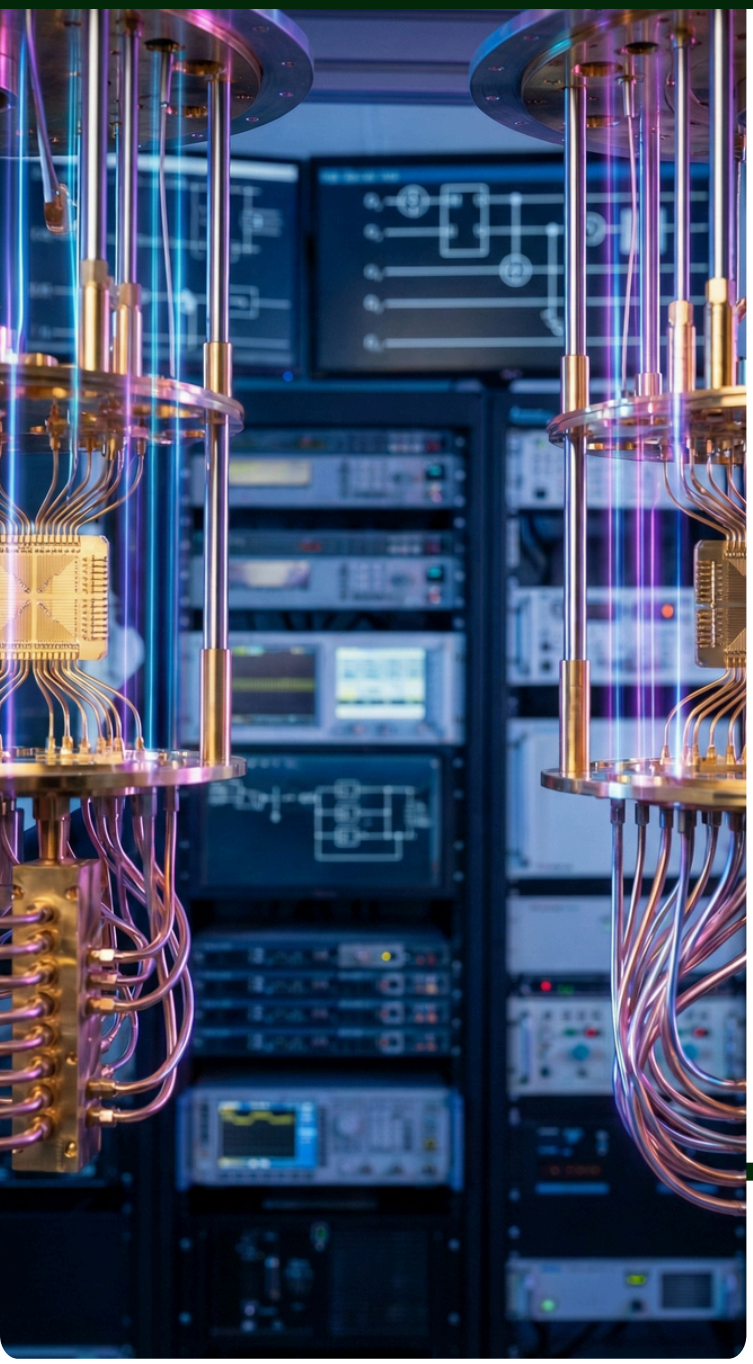
(Pasqal-IBM collaboration) ; (IBM-QCSC software / Slurm plugins)

In parallel, Pasqal is **expanding usage of its systems** through major **cloud access** (Microsoft Azure, Google Cloud Platform, etc.), enabling users to run workloads on its Quantum Processing Units via tools such as **NVIDIA CUDA-Q** for hybrid quantum-classical programming, and **NVQLink**, which aims at tighter QPU-GPU coupling. (Pasqal-NVIDIA CUDA-Q). Various challenges still remain such as **Interconnection & orchestration** (errors correction, scheduling, resource management, standardized interfaces, etc.).

Currently, the quantum market is largely driven by **on-premises hardware sales** from **publicly funded entities**. In this context, Pasqal stands out as a **clear leader**: the **company has won 3 out of 8 public tenders in Europe**, including **all public tenders dedicated to the installation of neutral-atom QPUs**. Pasqal is also the **company that has deployed the highest number of 100+ qubit QPUs** in **operational datacenters**, highlighting its strong **execution capabilities** and **technological maturity**.



From your experience, what does meaningful commercial adoption look like today, and how should organizations think about near-term value or ROI from quantum computing?



For Pasqal, meaningful commercial adoption encompass:

- **Large number** of **enterprise-grade quantum processing units delivered** or **hosted** (on-premises or through the cloud);
- **Structured and repeatable end users quantum usage** over time (use-case backlog, benchmarking vs classical);
- **Integration into real compute environment** (HPC/cloud/workflows).

Pasqal is a **deployment-first** quantum hardware player, delivering neutral atom QPUs into real infrastructures and scale execution through standardized systems allowed by off-the-shelf components, cloud access, and tight **HPC integration** – this is demonstrated through the multiple Quantum Processing Units Pasqal deployed:

European public procurement traction: Pasqal is a leading supplier in EuroHPC competitive procurements (e.g., on-prem systems integrated into Europe's first hybrid HPC-Quantum infrastructure and EuroHPC procurements), with public references deliveries such as **HPCQS deployments (CEA/TGCC + Jülich)** and **EuroQCS-Italy (CINECA)**.

(Pasqal – Europe's first hybrid HPC–Quantum infrastructure); (EuroHPC JU – EuroQCS-Italy procurement contract); (Pasqal – EuroQCS-Italy selection)

Industrial deployment at scale: Pasqal signed with **Aramco** to install, maintain, and operate a **200-qubit** system in Saudi Arabia, explicitly framed as an industrial program.
(Pasqal-Aramco Quantum Hardware deployment)

International industrialization: Pasqal expanded manufacturing with a **second quantum factory** in **Canada** in **Sherbrooke** (the first factory being in Paris, France), delivering a **Quantum Processing Unit to DistriQ**, fully manufactured and installed locally.
(Pasqal – Canada factory & DistriQ sale)

Taken together, these milestones reflect **both technology readiness and unique industrial delivery capability.**

How does Pasqal view the evolving Indian quantum ecosystem, and in what ways do you see Pasqal contributing to India's national priorities such as talent development, research collaboration, and real-world quantum applications?

India is building one of the most promising quantum ecosystems globally, with a clear ambition to connect **public strategy, HPC-scale infrastructure, research excellence**, and **application-led industrial outcomes**. A case in point is the **Amaravati Quantum Valley** initiative which already attracted a significant number of technology leaders such as IBM and TCS, as well as international and Indian startup companies.

Pasqal sees its contribution as **ecosystem enablement at scale** characterized by four levers aligned with national priorities:

1

Real-world applications

Supporting application programs that connect quantum with existing compute environments (HPC/cloud) and develop use cases fitting with India's industry priorities.

2

Research collaboration

Partnering with academic and research stakeholders on **quantum simulation** and **hybrid analog–digital** approaches-areas where neutral atom are particularly well suited, thus where India can convert fundamentals into publishable and reusable results.

3

Talent development

Accelerating workforce readiness via accessible tooling and structured pathways to help learners moving from experimentation to deployable workflows.

4

Supply Chain

Pasqal aims at contributing to the local quantum supply chain emergence, through collaboration with local manufacturers for local sourcing.

As quantum computing moves from research toward industrial adoption, how does Pasqal think about benchmarking, validation, and setting realistic expectations with partners?

Pasqal turns research into hardware. Pasqal's 2025 Quantum Roadmap articulates a bold strategy founded on unmatched engineering strength and structured around three pillars: **rapid deployment of enterprise-grade QPUs**, targeted **demonstrations of quantum advantage** and **accelerated progress toward scalable fault-tolerant systems**. In that sense, Pasqal systematically **benchmarks quantum results against state-of-the-art classical methods** to rely on clearly defined and measurable criteria within the Quantum Advantage framework. In practice, this translates into two principles:

Customer needs:
Pasqal aligns with partner's needs by focusing on specific problems and successes to be addressed using Quantum Computing rather than Classical methods.

Reproducible validation:
Pasqal relies on repeatable evaluation protocols and iterative testing (emulation capabilities and hardware runs) to ensure results are robust, comparable, and traceable over time.

As a case in point, **together with IBM, Pasqal** has developed a **robust approach** to **Quantum Advantage** by clarifying its definition and benchmarking against classical computation. This framework ensures that early engagements generate **credible, decision-useful evidence** to build durable foundations for scaling value as **quantum hardware, software, algorithms,** and **applications** continue to evolve.

SUPER COMPUTING INDIA 2025

Supercomputing India 2025 (SCI 2025) served as a premier national forum bringing together researchers, policymakers, industry leaders, and system architects to discuss the future of High Performance Computing (HPC), Artificial Intelligence (AI), and Quantum Computing in India. As India advances its ambitions under the National Supercomputing Mission (NSM) and the National Quantum Mission (NQM), SCI 2025 played a critical role in aligning technological progress with strategic objectives. A defining highlight of SCI 2025 is its growing emphasis on quantum computing as a natural extension of the supercomputing ecosystem, rather than a standalone technology. The conference reflects a clear shift toward hybrid computing architectures, where quantum processors complement classical supercomputers to address problems beyond the reach of conventional methods.

The significant milestone of Qniverse crossing 10k users was celebrated. Qniverse currently has over 13k users and has executed over 10k quantum simulations. In a field often constrained by limited hardware access, Qniverse's growth story illustrated how simulators and cloud platforms are becoming the training ground for the next generation of quantum developers and researchers.

Credits : Vikas Ramaswamy

159 Sessions

342 Speakers

8286 Attendees

5873 Delegates

187 Exhibitors

20 Countries

2413 Academicians

SCI 2025

“

Quantum computing is not a substitute for classical HPC; it is a specialized accelerator designed to integrate seamlessly with existing computational infrastructures.

This perspective aligns closely with the realities of near-term quantum hardware, which depends heavily on classical computing for control, compilation, error mitigation, and end-to-end workflow orchestration.

Discussions at the conference underscored that quantum advantage will arise through co-design, with algorithms, hardware, software, and system-level orchestration evolving in tandem- an approach that naturally aligns with the supercomputing community’s deep expertise in scalable systems engineering, performance optimization, and resource management.

The most visible marker of this shift was the keynote session on Quantum Computing in the Supercomputing Era. Rather than celebrating quantum machines in isolation, the keynote grounded the discussion in systems reality. Quantum processors were presented as accelerators embedded within HPC environments, dependent on classical supercomputers for compilation, scheduling, calibration, and error mitigation. This framing resonated strongly with the SCI audience, positioning quantum computing as a natural extension of the supercomputing stack rather than a parallel ecosystem. The momentum surrounding India’s National Quantum Mission (NQM) was clearly evident throughout the program. SCI 2025 became a platform where policy ambition translated into concrete progress.

A special focus was placed on the role of startups. SCI 2025 provided a crucial link for these emerging enterprises to connect with academic partners, and the larger HPC industry. This was directly supported by announced collaborations, such as the Memorandum of Understanding (MoU) between C-DAC and global quantum focused companies to explore co-development of hybrid quantum technologies and multiple panel discussions on quantum computing.

Credits: Vikas Ramaswamy

India's Quantum Leap - The NQM Perspective panel discussion examined how India's academic breakthroughs are transitioning into deployable assets under the National Quantum Mission, while "Global Quantum Synergy - Building Bridges from India to the World" explored and analyzed global quantum perspective and where India stands. Industry and ecosystem perspectives were captured in the Quantek Panel where founders and industry professionals discussed open quantum systems, commercialization pathways and talent pipelines. In HPC based Quantum Accelerators for Enabling Quantum Computing on Supercomputers panel discussion researchers from CDAC talked about how the existing HPC resources complement quantum accelerators. Complementing this, Hybrid Quantum-Classical Supercomputing Architectures: Bridging the Gap Between HPC and QPU offered a grounded discussion on timelines, benchmarks, and quantum use cases, deliberately steering away from hype. Together, these panels framed quantum computing at SCI 2025 as a co-ordinated, mission-driven effort spanning infrastructure, software, industry participation, and realistic deployment within the supercomputing stack.

Quantum focused companies from India and worldwide participated to showcase their developments in this emerging sector. Supercomputing India 2025 marks an important milestone in India's journey towards next-generation computing. By embedding quantum computing firmly within the supercomputing narrative, SCI 2025 advances a realistic and scalable vision where quantum systems enhance, rather than replace, classical HPC. Through keynotes, mission-aligned announcements, platform milestones, and ecosystem-building efforts, quantum computing was presented as an emerging operational layer of India's supercomputing strategy. SCI 2025 thus captured a moment where quantum moved decisively from curiosity to capability, firmly anchored within the nation's broader computational vision. As quantum technologies mature, SCI will continue to play a vital role in shaping an integrated computational ecosystem capable of addressing national and global scientific challenges.

Visit
sci25.supercomputingindia.org
for more Insights on
Transpired Events

Credits : Vikas Ramaswamy

SCI 2025 Gallery

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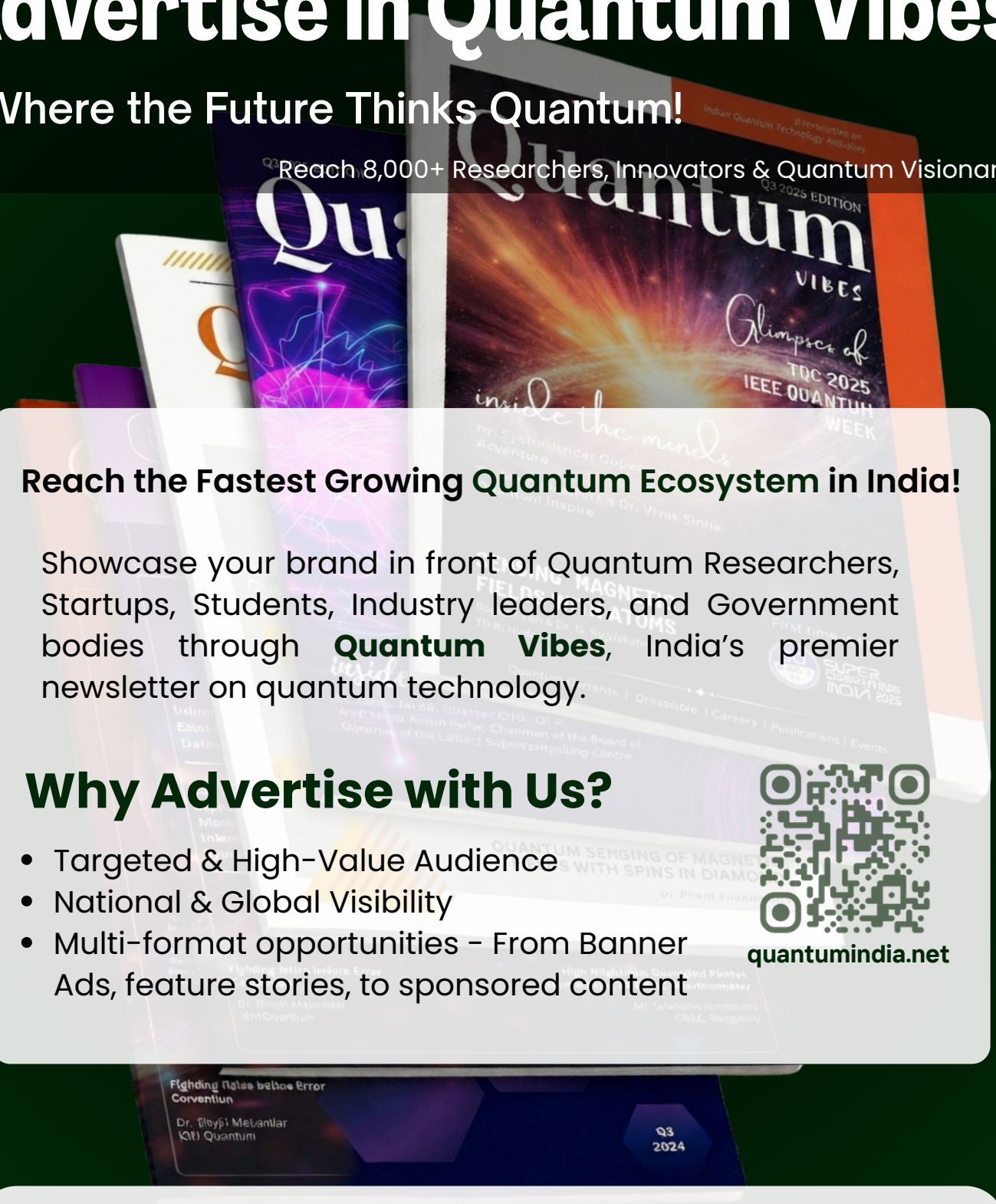

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Quantum Currents

From uncertainty to innovation - quantum breakthroughs are in motion.

01 OCTOBER 2025

BREAKTHROUGH IN CERTIFIED QUANTUM RANDOMNESS

Researchers from the Raman Research Institute (RRI) and IISc have successfully demonstrated "Certified Quantum Randomness" using a single qubit on a cloud-accessible, general-purpose quantum computer. Unlike traditional computers that use predictable rules, this quantum method provides a reliable source of true randomness. This breakthrough is pivotal for unhackable digital security and secure cryptographic keys, proving that true quantum advantages can be harnessed using current, noisy quantum processors.

The innovation lies in shifting from complex "separation in space" experiments to simpler time-based tests on a single unit of information. This allows quantum-certified outcomes to be generated without the need for specialized laboratory optical tables. The technique serves both as a tool for high-level encryption and as a benchmark to assess the precision and health of quantum hardware.

Source - PIB

12 NOVEMBER 2025

INDIA'S FIRST INDIGENOUS QUANTUM DIAMOND MICROSCOPE

Under the National Quantum Mission, the P-Quest Group at IIT Bombay has developed India's first indigenous Quantum Diamond Microscope (QDM). This breakthrough device utilizes Nitrogen-Vacancy (NV) centers in diamonds to enable high-resolution, three-dimensional magnetic field imaging at the nanoscale. The QDM has already secured India's first patent in this domain and was showcased at the Emerging Science Technology and Innovation Conclave (ESTIC 2025).

The microscope holds transformative potential for the semiconductor industry, as it can map magnetic fields in 3D layers within encapsulated chips - a feat traditional tools struggle to achieve. Beyond electronics, the QDM is expected to revolutionize neuroscience and materials research by allowing scientists to visualize dynamic magnetic activity at room temperature. Future versions will integrate AI and ML to further enhance computational imaging.

Source - PIB

05 NOVEMBER 2025

PM GIFTS PATHBREAKING INNOVATIONS AT ESTIC 2025

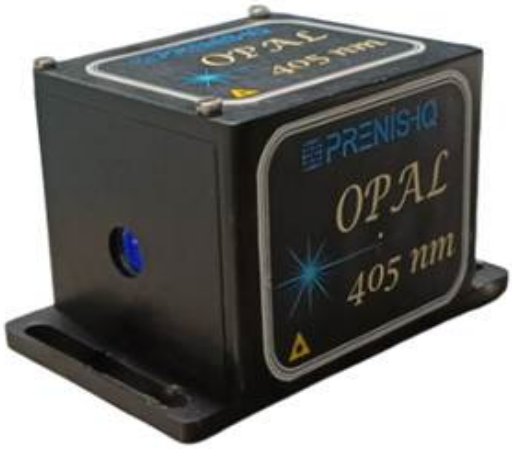
During ESTIC 2025, Prime Minister Narendra Modi gifted three landmark innovations to the nation: the QSIP (Quantum Security Chip), a 25-qubit QPU (Quantum Computing Chip), and NexCAR19. The 25-qubit QPU represents India's first full-stack indigenous quantum computing chip, combining scalable hardware and optimized software. These breakthroughs underscore India's rapid transition into a deep-tech powerhouse capable of solving once-uncomputable global challenges.

Alongside the quantum achievements, the Prime Minister highlighted NexCAR19, India's first indigenous CAR-T cell therapy for cancer. Developed by ImmunoACT (an IIT Bombay spin-off), this "living drug" offers a humanized treatment for leukemia that is significantly more affordable than global alternatives. Supported by the Department of Biotechnology and BIRAC, this therapy showcases the success of the Indian startup ecosystem in delivering world-class, life-saving medical technology.

Source - PIB

14 NOVEMBER 2025

INDIGENOUS HIGH-PRECISION DIODE LASER FOR QUANTUM TECH



Prenishq Pvt Ltd, an IIT Delhi spin-off supported by the National Quantum Mission, has launched India's first indigenous high-precision compact diode laser. These lasers are essential enablers for quantum encrypted communication and photonic quantum computing. By delivering exceptional beam stability and quality across various wavelengths, the device allows for the precise control of qubits necessary for advanced scientific research and secure financial transactions.

The laser is designed to be a "plug-and-play" solution with low power consumption and high efficiency, making it ideal for both research labs and industrial integration. Its development aligns with the national goal of becoming a global leader in manufacturing quantum technology products. The project received multi-agency support, including from the DST-Nidhi Prayas and various Technology Innovation Hubs across India.

Source - PIB

24 NOVEMBER 2025

₹720-CRORE QUANTUM FABRICATION FACILITIES

Union Minister of State (Independent Charge) for Science & Technology, Dr. Jitendra Singh announced the establishment of four state-of-the-art Quantum Fabrication and Central Facilities worth ₹720 crore at IIT Bombay, IISc Bengaluru, IIT Kanpur, and IIT Delhi. These facilities are designed to indigenize the production of quantum computing chips using superconducting, photonic, and spin qubits and quantum sensors. This move significantly reduces India's dependence on foreign laboratories and creates a foundational hardware ecosystem for sovereign technological growth.

These centralized hubs will be accessible to researchers, startups, and industry players nationwide to fast-track prototyping and small-scale production. Beyond hardware, the minister also highlighted the "BharatGen" initiative, India's first sovereign multilingual AI model project. Together, these missions reflect a "democratization of science" aimed at making deep-tech innovation accessible to rural innovators and established institutions alike.

Source - PIB

04 DECEMBER 2025

NITI AAYOG'S QUANTUM ECONOMY ROADMAP

NITI Aayog's Frontier Tech Hub, in collaboration with IBM, has released a comprehensive roadmap titled "Transforming India into a Leading Quantum-Powered Economy." The roadmap outlines a strategic 10-year vision to integrate quantum computing, secure communication, and precision sensing into national missions. It emphasizes building globally competitive platforms and high-value software services to ensure India becomes a global supplier of quantum technology rather than just a consumer.

The initiative highlights that the next five years are critical for scaling India's domestic hardware and software capabilities. By leveraging the existing National Quantum Mission, the roadmap identifies key interventions to accelerate R&D and commercialization. It also focuses on nurturing specialized talent and creating a resilient digital infrastructure that can redefine sectors like healthcare, finance, and national security.

Source - PIB

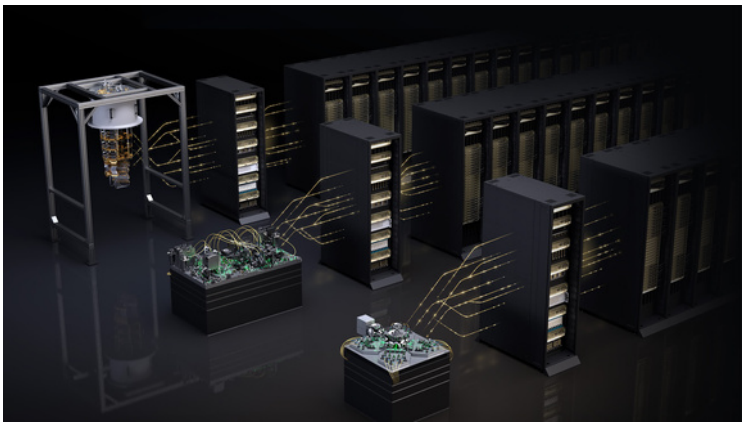
INTERNATIONAL QUANTUM NEWS

28 OCTOBER 2025

NVQLINK UNVEILED: BRIDGING GPUS AND QUANTUM PROCESSORS FOR HYBRID SUPERCOMPUTING

In late October 2025, NVIDIA formally unveiled NVQLink, a new open system architecture designed to tightly connect quantum processors with high-performance GPUs. This initiative brings together 17 quantum hardware builders and multiple leading scientific supercomputing centers, including U.S. national labs, under a unified approach to hybrid classical-quantum computing. By enabling low-latency, high-throughput communication between GPUs and QPUs, the platform aims to accelerate research areas such as quantum error correction, materials simulation, and next-generation chemistry applications.

The significance of NVQLink lies in its intent to dissolve the traditional silos between HPC and Quantum Computing stacks. Rather than treating quantum processors as distant experimental devices, NVIDIA's architecture embeds them within familiar GPU-accelerated workflows, so that classical and quantum layers can interact in real time. This lays a technical foundation for future hybrid systems that may tackle problems beyond the reach of either classical HPC or standalone quantum machines.



Source - NVIDIA Newsroom

12 NOVEMBER 2025

ENGINEERING TOWARD ADVANTAGE: IBM QUANTIFIES THE ROAD TO FAULT-TOLERANT QUANTUM COMPUTING

In November 2025, IBM detailed a decisive step forward in its quantum roadmap, unveiling new processors, software upgrades, and algorithmic benchmarks aimed squarely at achieving quantum advantage. At the hardware level, IBM introduced Quantum Nighthawk, a 120-qubit superconducting processor equipped with 218 tunable couplers, enabling 30 percent higher circuit complexity than previous generations. The system is designed to reliably execute circuits containing up to 5,000 two-qubit gates, with a clear scaling trajectory toward 7,500 gates in 2026, 10,000 in 2027, and 15,000 by 2028 as connectivity and coherence improve.

Equally significant were advances toward fault tolerance. IBM reported a breakthrough in real-time error-correction decoding, achieving latency below 480 nanoseconds, nearly 10× faster than earlier leading methods and delivered one year ahead of schedule. On the software side, enhancements to Qiskit improved algorithmic accuracy by 24 percent on systems exceeding 100 qubits, while new execution and error-mitigation techniques reduced computational cost by more than 100× when paired with classical HPC resources. Backed by a transition to 300 mm quantum wafer fabrication, enabling 10× higher chip complexity, IBM reaffirmed its targets of verifiable quantum advantage by 2026 and a large-scale fault-tolerant quantum computer by 2029, setting one of the industry's most quantitatively defined quantum timelines.

Source - IBM Newsroom

24 NOVEMBER 2025

SAUDI ARABIA ENTERS THE QUANTUM ERA WITH FIRST INDUSTRIAL-GRADE SYSTEM

In a historic leap for the Middle East's tech landscape, Saudi Aramco and Pasqal announced the deployment of Saudi Arabia's first quantum computer, housed at Aramco's Dhahran data center. Powered by Pasqal's neutral-atom platform, the system controls 200 qubits in programmable two-dimensional arrays, marking the region's first industrial quantum computer dedicated to real-world applications across energy, materials, and industrial sectors.

The milestone reflects both Saudi Arabia's strategic move into advanced computing and Aramco's ongoing digital transformation strategy, which integrates AI and next-generation technologies to enhance operational efficiency and innovation. Beyond the hardware itself, the partnership includes training programs and joint research opportunities to cultivate local expertise, signaling a broader effort to build a regional quantum ecosystem and nurture high-tech talent within the Kingdom. Pasqal's CEO described the deployment as a "landmark for the Middle East's quantum future," underscoring the global importance of this development.

Source - IBM Newsroom

25 NOVEMBER 2025

QUANDELA AND OVHCLOUD LAUNCH MERLIN TO DEMOCRATIZE QUANTUM MACHINE LEARNING

In Paris at the Adopt AI event in late November, Quandela and OVHcloud announced a strategic collaboration to bring quantum machine learning into broader research and industry practice. Their initiative centers on MerLin, a programming framework dedicated to hybrid quantum-classical machine learning, which will be made available through OVHcloud's cloud platform starting mid-2026. MerLin is positioned to let developers prototype and simulate models on GPUs before scaling to photonic quantum hardware, effectively lowering the entry barrier for quantum-enhanced AI experimentation.

This partnership emphasizes two key trends in the quantum ecosystem: the rise of application-focused quantum software, and the integration of quantum capabilities within sovereign cloud environments. By combining Quandela's expertise in photonic quantum processors with OVHcloud's infrastructure, the collaboration aims to nurture a European-centric quantum machine learning community while also providing global access to emerging hybrid workflows.

Source - Quandela & OVHcloud Announcement

22 DECEMBER 2025

USTC'S ZUCHONGZHI 3.2 CROSSES CRITICAL QUANTUM ERROR CORRECTION THRESHOLD

In late December 2025, researchers at the University of Science and Technology of China reported that their superconducting quantum processor Zuchongzhi 3.2 had achieved quantum error correction below the surface-code threshold, a central requirement for scalable, fault-tolerant quantum computing. The system comprises 107 frequency-tunable transmon qubits arranged in a 2D square lattice with nearest-neighbour connectivity. Using an all-microwave control and leakage-suppression architecture, the team realized a surface-code logical qubit at distance 7, demonstrating that the logical error rate decreases as code distance increases instead of rising a defining signature of operation below the error correction threshold. The experiment measured an error-suppression factor ≈1.40, confirming that adding more physical qubits improves logical performance and that error correction stabilizes the computation rather than degrading it.

This breakthrough tackled one of the most stubborn hurdles in fault-tolerant designs: quantum state leakage and correlated errors that arise when qubits drift out of their intended computational states. By using carefully timed microwave pulses for both leakage suppression and fast unconditional reset of ancilla qubits, the Zuchongzhi 3.2 team reduced average leakage by roughly 70× compared with unsuppressed operation, while maintaining high-fidelity readout (~0.95% error) within typical readout windows (~300 ns). The result places China among only a very small group of research teams worldwide to demonstrate error correction that genuinely suppresses errors as system size scales, a key step toward building fault-tolerant quantum computers with millions of physical qubits.

Source - Physical Review Letters (Via Quantum Computing Report by GQI)

A career in quantum isn’t just a job - it’s a chance to shape how the future computes

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5 D-Wave Manager, Quantum Processor Development Hybrid (Burnaby, British Columbia, CA)	**6** Infleqtion Principal Electrical Engineer - Team Lead Louisville, Colorado, United States	**7** PsiQuantum Photonics Engineer Palo Alto, California, United States	**8** Atom Computing Quantum Engineer Boulder, CO
9 Accenture Quantum Security Lead (Cryptography/NIST PQC) Kuala Lumpur	**10** Quandela Senior Research Program Lead Washington, District of Columbia, United States	**11** Atom Computing Senior Software Engineer - Control Systems Boulder, CO or Austin, TX	**12** Quandela HPC Integration & Support Engineer Bruyères-le-Châtel, Île-de-France, France
13 PsiQuantum Quantum Applications Software Developer Daresbury, England, United Kingdom, Palo Alto, California, United States, Remote	**14** Quandela Application & Algorithm Support Engineer - Quantum Computing (HPC Context) Bruyères-le-Châtel, Île-de-France, France	**15** Oak Ridge National Laboratory Postdoctoral Research Associate - Quantum Algorithms for Materials Simulations Oak Ridge, TN, US	**16** QubitSolve Quantum Software Engineer Morgantown, WV

QUANTUM TECHNOLOGY CONFERENCES AND WORKSHOP

January - March 2026

JAN 17 - JAN 22

SPIE Quantum West

San Francisco, United States

JAN 05 - JAN 09

55th Winter Colloquium on the Physics of Quantum Electronics (PQE 2026)

Snowbird, United States

JAN 24 - JAN 30

Quantum Information Processing Conference (QIP2026)

Riga, Latvia

FEB 03 - FEB 05

International Conference on Nanoscience and Nanotechnology (ICONN2026)

Sydney, Australia

MAR 01 - MAR 07

NanoLight 2026

Benasque, Spain

MAR 05 - MAR 07

Quantum Artificial Intelligence & Optimization 2026 (QAIO 2026)

Marbella, Spain

MAR 06 - MAR 07

Third International Conference on Quantum AI and Deep-Tech Innovations for Next-Gen Intelligence (QUADNEXT-2026)

Agiripalli, India

MAR 09 - MAR 12

Concepts of Quantum and Spacetime

Tsukuba, Japan

MAR 11 - MAR 13

International Conference on Materials for Electronics, Energy, Quantum and Biomedical Technologies (mqubit2026phy)

Madurai, India

MAR 12 - MAR 13

1st National Conference on Quantum Materials and Devices (NCQMD2026)

Raipur, India

MAR 16 - MAR 20

Quantum Resources 2026

Tokyo, Japan

MAR 24 - MAR 26

Third International Conference on Trends in Quantum Computing and Emerging Business Technologies 2026 (TQCEBT 2026)

Pune, India

RECENT PUBLICATIONS IN QUANTUM TECHNOLOGIES

October - December 2025

October 2025

Optimal adaptation of surface-code decoders to local noise

Phys. Rev. A 112, 042431

Andrew S. Darmawan

November 2025

Characterizing transport in a quantum gas by measuring Drude weights

Science, Vol 391, Issue 6782

Philipp Schüttelkopf, Mohammadamin Tajik, Nataliia Bazhan, Federica Cataldini, Si-Cong Ji, Jörg Schmiedmayer, and Frederik Møller

November 2025

Fast mixed-species quantum logic gates for trapped-ion quantum networks

Phys. Rev. A 112, L050601

Zain Mehdi, Varun D. Vaidya, Isabelle Savill-Brown, Phoebe Grosser, Alexander K. Ratcliffe, Haonan Liu, Simon A. Haine, Joseph J. Hope, and C. Ricardo Viteri

November 2025

Feedforward suppression of readout-induced faults in quantum error correction

Phys. Rev. A 112, L050602

Liran Shirizly, Dekel Meirom, Malcolm Carroll, and Haggai Landa,

December 2025

Hardware-Efficient Quantum Phase Estimation via Local Control

PRX Quantum 6, 040348

Benjamin F. Schiffer, Dominik S. Wild, Nishad Maskara, Mikhail D. Lukin, and J. Ignacio Cirac

December 2025

Local clustering decoder as a fast and adaptive hardware decoder for the surface code

Nature Communications volume 16, Article number: 11048 (2025)

Abbas B. Ziad, Ankit Zalawadiya, Canberk Topal, Joan Camps, György P. Gehér, Matthew P. Stafford & Mark L. Turner

December 2025

All You Need is pi: Quantum Computing with Hermitian Gates

Quantum, volume 9, page 1925

Ben Zindorf and Sougato Bose

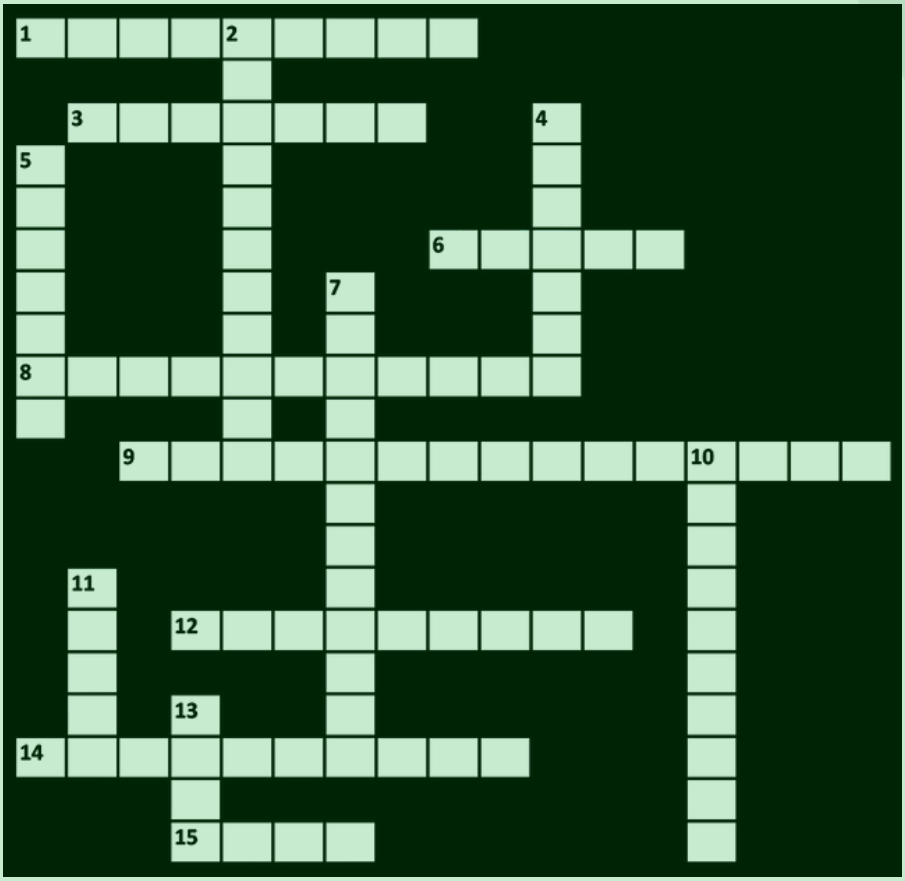
December 2025

Experimental Quantum Error Correction below the Surface Code Threshold via All-Microwave Leakage Suppression

Phys. Rev. Lett. 135, 260601

Tan He, Weiping Lin, Rui Wang, Yuan Li, Jiahao Bei, Jianbin Cai, Sirui Cao, Danning Chen, Kefu Chen et al.

QROSSWORD



Top early solvers will be featured in the next edition of

QUANTUM VIBES MAGAZINE!

Across

1. Quantum computing approach where information is carried by individual light particles
3. Periodic light structure used to arrange atoms in quantum experiments
6. Smallest unit used to store quantum information
8. Quantum platform based on atoms with no net electric charge
9. Quantum platform where electrical current flows with zero resistance
12. Light quanta that act as information carriers in optical quantum systems
14. Cooling science used to reach temperatures near absolute zero
15. Quantum platform that encodes information in intrinsic particle rotation

Down

2. Light-based structure used to confine neutral atoms
4. Common metal used to fabricate superconducting quantum circuits
5. Solid material hosting atomic-scale defects for quantum control
7. Orientation property of light used in optical quantum systems
10. Quantum computing approach that uses electrically charged atoms
11. Light-based tool used to slow and cool atoms in quantum experiments
13. Charged atoms confined using electromagnetic fields

Q3 2025 Answers

1. Unitary
2. Hamiltonian
3. Photon
4. Oracle
5. Superposition
6. Shors
7. Superconducting
8. Grover
9. Teleportation
10. Entanglement
11. Bitflip
12. Heisenberg
13. Ground
14. Measurement
15. Qubit
16. NoCloning
17. Simon
18. Hilbert
19. Diffusion
20. Ancilla

Q3 2025 Early Solvers

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Share your Crossword solution with us at quantum-outreach-blr@cdac.in

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