# VIGYAN 2047

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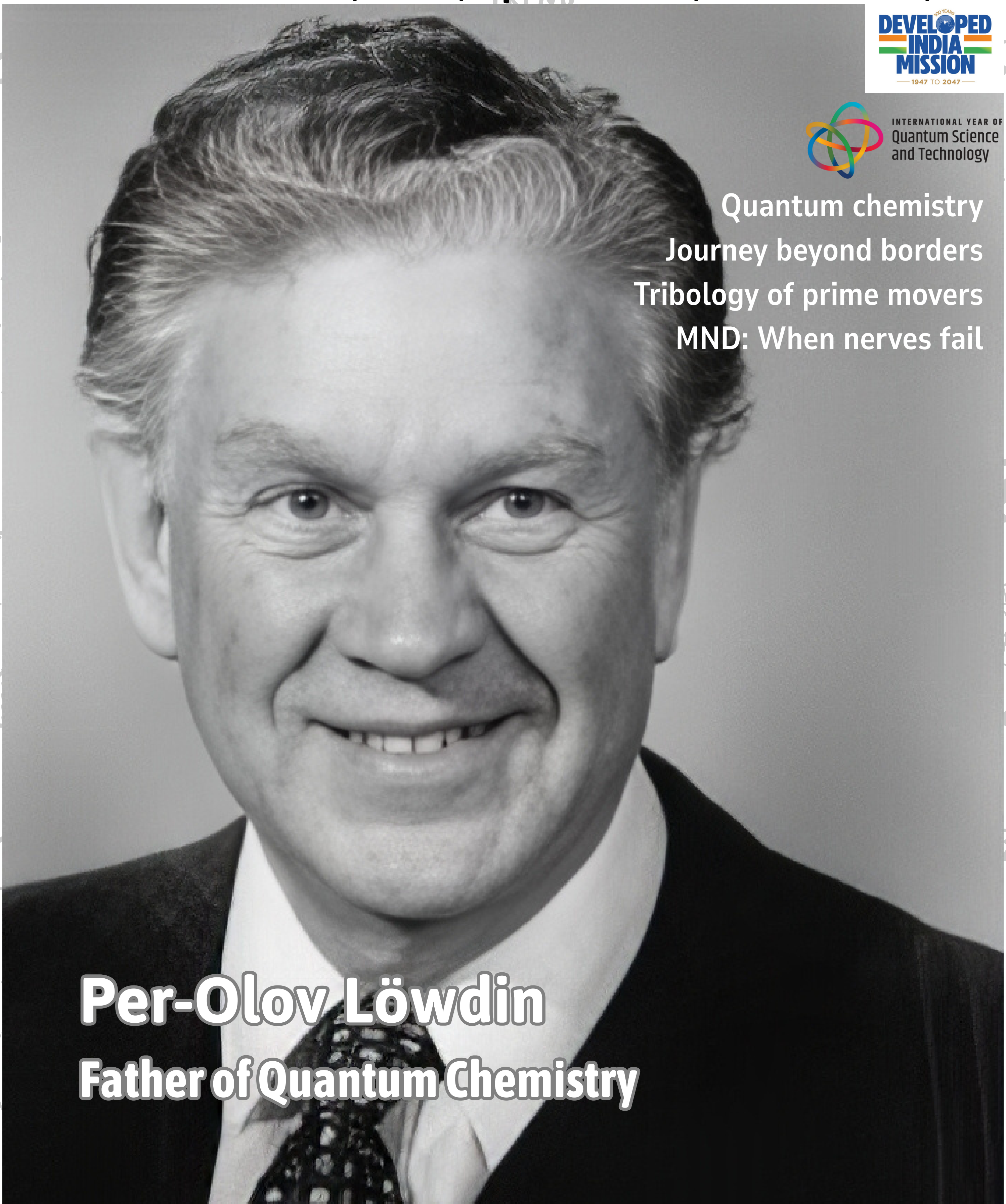
DEVELOPED INDIA MISSION
1947 TO 2047

INTERNATIONAL YEAR OF Quantum Science and Technology



Quantum chemistry

Journey beyond borders

Tribology of prime movers

MND: When nerves fail

## Per-Olov Löwdin

### Father of Quantum Chemistry

**VIGYAN 2047**

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# In This Issue




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# Letter to the editor

Dear Editor,
I recently obtained the latest edition of Vigyan 2047, the special issue dedicated to Acharya P.C. Ray. It was truly enlightening to learn so much about his life, his scientific contributions, and how he rose to the clarion call from Tata Steel to produce much-needed chemicals for it steel production.
The timing of this edition could not have been more apt. Today, once again, we Indians must respond to the call for self-reliance and strengthen our economy to make it more robust than ever before. As your magazine so rightly emphasizes, science has always been, and will continue to be, the answer to these challenges.
I sincerely thank you and your team for spreading awareness through this valuable monthly initiative. Kudos to Vigyan 2047 for keeping the spirit of science communication alive.
Warm regards,
Mohd. Nadeem, Hapur

# Editorial

## A Legacy of Light and Quantum Vision

**Prof. Zahid Hussain Khan** has been a physicist par excellence—not merely because he introduced me, over four decades ago, to the intricacies of **optics, spectroscopy, and lasers,** but because of his unyielding dedication to spreading scientific awareness across borders and generations. What sets him apart is not just his mastery of Physics, but his relentless mission to ensure that science, especially in the domains of light and quantum technologies, reaches the masses.

For years now, Prof. Khan has been at the forefront of promoting **science outreach,** championing events like the **International Day of Light** with remarkable consistency. He has weathered challenges—logistical, personal, and institutional—but never once has he faltered in his commitment to public science engagement. Through **eloquent lectures, insightful writings, and grassroots outreach,** he has ignited curiosity and deepened understanding among students, educators, and lay audiences alike.

Most recently, in collaboration with **Prof. John Dudley**—renowned physicist and Chair of the Steering Committee of the International Year of Light—Prof. Khan organized a thought-provoking **seminar on Quantum Science & Technology.** We had the privilege of covering this event in our **July issue** of *Vigyan 2047,* and it received warm appreciation from our readers.

Yet Prof. Khan didn't stop there. As we moved into the commemorations of the **International Year of Quantum Science and Technology,** we requested him to contribute a **series of feature articles** for *Vigyan 2047,* aimed at making complex quantum concepts accessible to the wider public. True to form, he graciously accepted.

As this series began to take shape, we invited Prof. Khan to share some **personal recollections**—snippets from his journey through the world of Physics. That was when he revisited his formative interactions with **Prof. Per-Olov Löwdin,** the iconic founder of quantum chemistry. What followed was a touching and intellectually rich **memoir,** reflecting not only the brilliance of Prof. Löwdin but also the enduring mentorship and inspiration that shaped Prof. Khan's own scientific journey.

We are proud to present that memoir in this issue—an intimate glimpse into a golden era of quantum discovery, written with the warmth and insight that only a true disciple of science can offer.

As editor, I believe this edition holds something unique. It connects **past and future, memory and momentum, individual experience and global movement.** I invite our readers—scientists, students, teachers, and curious minds—to read, reflect, and share. Let this edition be not just an archive, but a catalyst.

If *Vigyan 2047* is to become the voice of India's scientific aspirations and its global collaborations, it is through such narratives—stories that resonate across national boundaries and scientific generations.

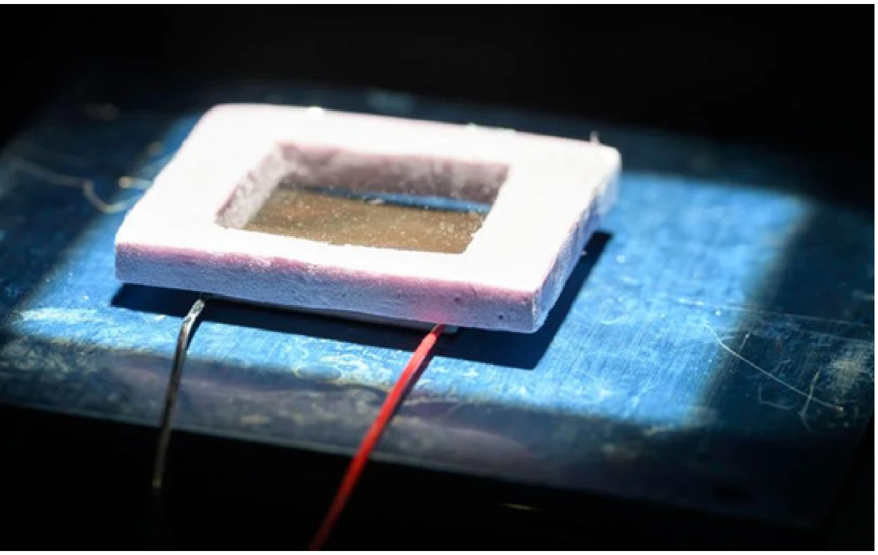
I urge you to help us take this message forward. Share this issue, recommend it to your peers, and let us ensure that **science reaches every doorstep**—not only in India, but around the world.

**Nakul Parashar,** PhD
nakul@shantifoundation.global

In The News

# New device generates 15x more electricity

Researchers exploring solar thermoelectric generators (STEGs) as an alternative to traditional solar panels have long faced a major hurdle: low efficiency. Unlike photovoltaic cells, STEGs generate electricity using



the Seebeck effect by creating a temperature difference between a hot and cold side. However, most STEGs convert less than 1% of sunlight into electricity, compared to about 20% for standard solar panels. A team at the University of Rochester dramatically improved STEG efficiency—boosting power output by 15 times—without altering the semiconductor materials. Instead, they enhanced energy absorption and heat management. On the hot side, they used femtosecond lasers to create nanoscale structures on tungsten, turning it into a "black metal" that absorbs more solar energy. They then added a plastic cover to trap heat, mimicking a greenhouse. On the cold side, they treated aluminum to improve heat dissipation through radiation and convection. Their upgraded STEG successfully powered LEDs and could support wireless sensors, wearable tech, or off-grid systems in rural areas. The study was published in *Light: Science and Applications*. ◆

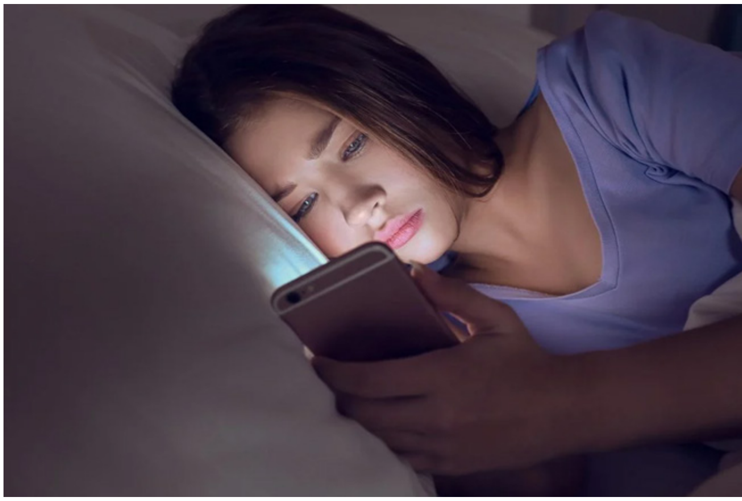
# New moth species discovered

A vividly colored moth long mistaken for a known species has now been identified as entirely new. Entomologist Dr. Peter Huemer of the Tyrolean State Museum in Innsbruck, Austria, described the

species in *Alpine Entomology,* naming it *Carcina ingridmariae* in honor of his wife on their 42nd wedding anniversary. Despite its striking pink and yellow hues, the moth was overlooked for over a century due to its close resemblance to the widespread oak carcina (*Carcina quercana*), first recorded in 1775. The breakthrough came with DNA barcoding, which revealed over 6% genetic divergence between the two species. Follow-up anatomical studies of reproductive structures confirmed the finding. The moth, about 2 cm in wingspan, is found across the eastern Mediterranean, including Greece, Croatia, Turkey, and Cyprus. Its caterpillars likely feed on oak trees, similar to its sister species, but more research is ongoing. Dr. Huemer, who has described over 200 European species in his 35-year career, called it "the prettiest species" he's ever encountered, making the name dedication an "obvious" choice. ◆

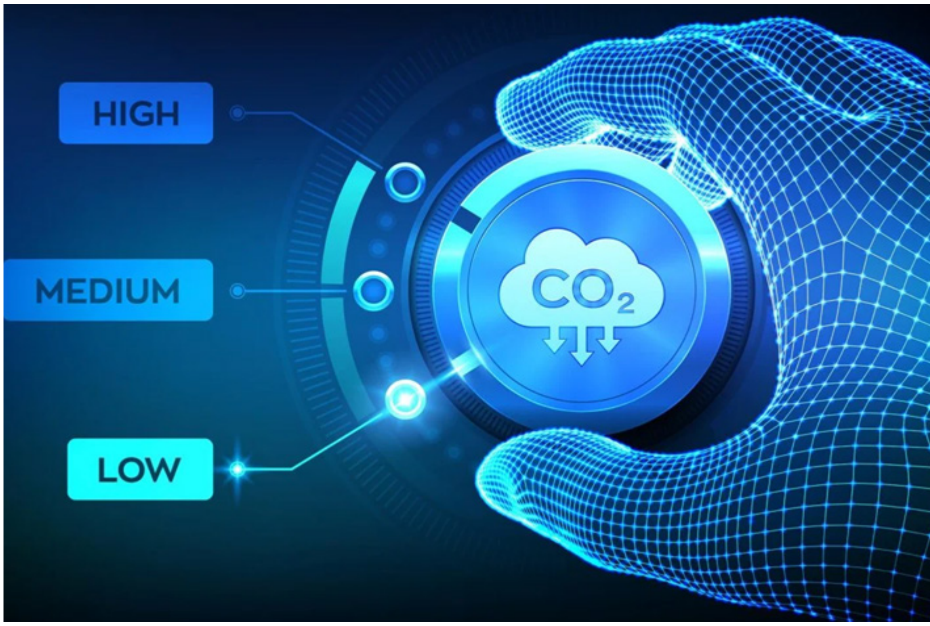
# Long screen time is bad for kids' hearts

Spending long hours on phones, computers, or gaming devices may increase the risk of developing cardiometabolic problems, such as high blood pressure, insulin resistance, and elevated cholesterol, according to a new study published in the Journal of the American Heart Association. Researchers analyzed data from over 1,000 Danish children and teens and found that more recreational screen time was linked to increased cardiometabolic risk. Each additional hour of screen time raised risk scores by 0.08 standard deviations in 10-year-olds and 0.13 in 18-year-olds. Lead author Dr. David Horner of the University of Copenhagen said even small increases add up over time, especially in youth spending three or more hours on screens daily. The study also found that shorter sleep duration and later bedtimes worsened the effects of screen time. Using machine learning, researchers identified a unique metabolic "fingerprint" in the blood associated with screen use, suggesting early biological changes. Experts recommend sleep-focused screen limits and parental modeling of healthy habits. While observational, the study highlights screen time as an important factor in early heart health.



# Hidden Cost of Smart AI

German researchers have found that AI models designed for step-by-step reasoning can emit up to 50 times more $CO_2$ than models that provide short, direct answers. Published in *Frontiers in Communication,* the study tested 14 large language models (LLMs) across 1,000 standardized questions. Models that "think" before responding generated an average of 543.5 internal tokens per question, compared to 37.7 from concise models—leading to much higher emissions without always improving accuracy. The most accurate model, Cogito (70 billion parameters), achieved 84.9% accuracy but emitted three times more $CO_2$ than similar-sized concise models. The study found an "accuracy-sustainability trade-off," with no low-emission models exceeding 80% accuracy. Subjects like abstract algebra and philosophy produced up to six times more emissions than simpler topics. Lead author Maximilian Dauner emphasized that users can lower emissions by choosing efficient models and prompting for concise answers. For example, DeepSeek R1 answering 600,000 questions emits the same $CO_2$ as a round-trip flight from London to New York. Raising awareness of AI's environmental cost could help promote more responsible use.



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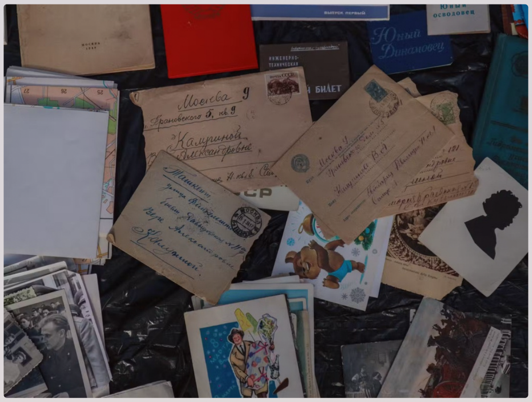
# A Journey Beyond Borders

## My Memoir of the 1975 Summer Institute in Quantum Chemistry, Solid State Physics, and Quantum Biology

*Zahid H Khan*

In 1975, shortly after submitting my Ph.D. thesis in Physics at Aligarh Muslim University, I found myself at a meaningful crossroads. With curiosity in my heart and time at my disposal, I came across an advertisement in a scientific magazine in the departmental seminar library about an "International Summer Institute in Quantum Chemistry, Solid State Physics, and Quantum Biology," to be held in Sweden and Norway.I applied by postal mail—an era when Air Mail envelopes and weeks of waiting defined global communication. Several weeks later, I received an acceptance letter from the organizers of the Summer School, awarding me a SIDA Fellowship. The fellowship covered all my travel expenses within Scandinavia. I only had to initially arrange funds for my air ticket, which would be reimbursed later. With support from my father, I arranged the funds and acquired a passport, an arduous task at the time, made possible through the help of a relative in Lucknow, whom I luckily met at the airport.

My confirmed ticket from Delhi to Stockholm had multiple layovers: Delhi – Kuwait – Cairo – Copenhagen – Stockholm. The return journey was rerouted as Oslo – Copenhagen – Delhi by the Summer Institute's official travel agent to make it more efficient. I applied by postal mail—an era when Air Mail envelopes and weeks of waiting defined global communication. Several weeks later, I received an acceptance letter from the organizers of the Summer School, awarding me a SIDA Fellowship. The fellowship covered all my travel expenses within Scandinavia. I only had to initially arrange funds for my air ticket, which would be reimbursed later. With support from my father, I arranged the funds and acquired a passport, an arduous task at the time, made possible through the help of a relative in Lucknow, whom I luckily met at the airport.



*Communication in the 1970s required patience and physical mail -- a stark contrast to today's instant connectivity.*

**Application**

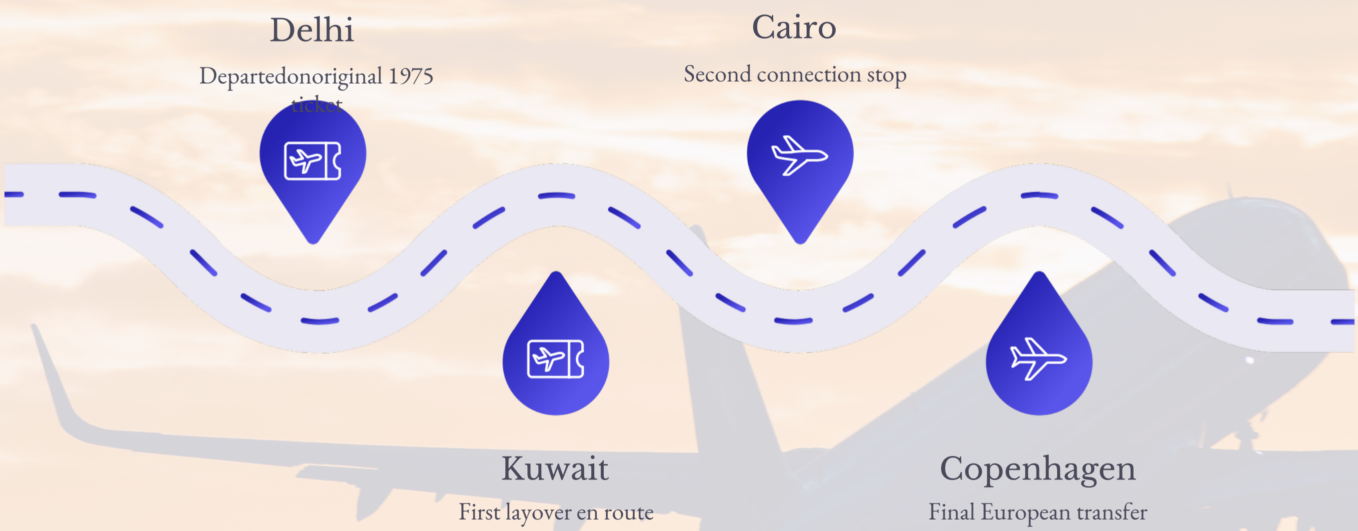
Applied via postal mail for the International Summer Institute.

**Acceptance**

Received a SIDA Fellowship covering all Scandinavian travel expenses.

**Preparation**

Arranged funds with father's support and acquired a passport.




At Copenhagen airport, I was the last passenger to board the connecting flight to Stockholm—my name echoed through the terminal. Unfortunately, my suitcase did not make it. After reporting the loss, I boarded the underground train and waited for a taxi. An elderly lady offered to share the ride, though it later turned out our destinations were different. The taxi driver, understanding my confusion, not only arranged another taxi for me but said words that still echo in my heart: *"Gentleman, since you are coming to this country for the first time, I will not charge you."*

The next morning, I boarded a train from Stockholm to Smedjebacken. The rail ticket had already been sent to me by post—another thoughtful gesture by the organizers.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## Smedjebacken: A Gentle Beginning

Our journey began with a warm welcome in Smedjebacken, a picturesque Swedish town. Participants had come from across Europe, South and West Asia, and the Asia-Pacific. Professor Per-Olov Löwdin and his trusted Ph.D. student, Dr. Michael Hehenberger, greeted us with genuine warmth.

At the formal welcome ceremony, the town's Mayor greeted each participant and presented with a red wooden horse—a traditional Swedish souvenir. A visit to a nearby farm gave us a taste of Swedish rural hospitality: fresh milk, bread, honey, and, unexpectedly, a personal library—leaving us to reflect on the cultural values often lacking in rural communities back home.

*Smedjebacken (Credit: https://www.smedjebacken.se/)*

Professor Löwdin and his wife Karin hosted us at their riverside ancestral home. We marvelled at his horses, personal boat, and above all, his pride in winter horse-riding on frozen rivers—a passion he claimed made him the only quantum chemist in Sweden to do so! The evening was filled with joyful dancing, deep discussions, and unforgettable Swedish cuisine.

Dr. Michael Hehenberger was a model of care and efficiency. He ensured that each participant felt welcome and looked after. Both he and Professor Löwdin would personally visit our motel, checking if we had letters to send home. Their humility left an indelible mark on all of us.

## Professor Per-Olov Löwdin: Architect of Global Quantum Discourse

Professor Löwdin was a towering figure in quantum science. He held dual appointments as professor—at Uppsala University in Sweden and as Head of the Quantum Theory Project at the University of Florida, Gainesville. He founded the International Journal of Quantum Chemistry and edited the prestigious series *Advances in Quantum Chemistry.* He also served on the Nobel Committee for Physics—a position of great influence.

## Uppsala University: The Academic Heart of the Institute

The Summer Institute's academic programme began at Uppsala University. Professor Löwdin opened with a chalk sketch of a tree—its roots were curiosity, its trunk science, and its branches the disciplines of physics, chemistry, and biology. At the canopy, he drew their convergence.

He explained the inclusion of Quantum Biology in the Summer Institute's scope with prophetic words: *"Man has explored the Earth and the sky but not yet understood himself. The 21st century will be the century of biological sciences."*

While discussing the organization of the International-level Summer Institute—held regularly over many years—Professor Löwdin spoke of the immense effort it required. He emphasized the need for strong connections with relevant ministries in the Swedish Government to ensure its continued success.

In an informal conversation, Professor Löwdin also confided that initially certain scientists had deliberately avoided citing his research in their publications. To counter this, he assembled a team of scholars who would refer his work in their own publications, helping to establish its visibility within the international scientific community. At the time, we were too young to fully grasp the implications, but as we matured, we began to recognize similar type of professional jealousy and disregard among scientists in our own countries as well.

Löwdin's lectures—delivered without notes, using only chalk and a blackboard—were intellectually profound and conceptually seamless. In the span of an hour, he would cover multiple blackboards with intricate derivations. From elegant treatments of Schrödinger's equation to the complexities of many-body theory and

*Group Photograph of Participants in the1975 Summer Institute, University of Uppsala, Sweden. (Credit: Uppsala Quantum Chemistry Group)*

### Teaching Excellence

Löwdin's lectures4delivered without notes, using only chalk and a blackboard4were intellectually profound and conceptually seamless. In the span of an hour, he would cover multiple blackboards with intricate derivations.

### Advanced Topics

From elegant treatments of Schrödinger's equation to the complexities of many-body theory and quantum coherence, the clarity and sophistication of his thinking were truly captivating.

### Innovative Approaches

A memorable highlight was his original derivation of Schrödinger's equation based purely on algebraic principles4 an innovative and intellectually stimulating approach that left a lasting impression on the audience.

quantum coherence, the clarity and sophistication of his thinking were truly captivating.

In his sessions, Professor Löwdin explored advanced topics such as orthogonalization techniques, extended Hartree-Fock theory, and density matrix methods. A memorable highlight was his original derivation of Schrödinger's equation based purely on algebraic principles—an innovative and intellectually stimulating approach that left a lasting impression on the audience. He also ventured into philosophical reflections, addressing the nature of objectivity and the foundational concepts underpinning quantum theory.

## Distinguished Faculty and Inspiring Lectures

Prof. Löwdin maintained high standards when selecting lecturers for the Summer Institute. He explicitly stated that applicants should consider applying only if they were proficient in both mountaineering and soccer.

Thus the Summer Institute featured the following extraordinary lineup of scientists:

### Prof. Jean-Louis Calais

Associate Director of the Institute and Professor of Quantum Chemistry at Uppsala. His lectures offered a clear exposition of molecular orbital theory and group symmetry, illustrating how symmetry principles streamline the analysis of electronic structure.

### Prof. Ruben Pauncz

A theoretical chemist from the Technion, Israel, Pauncz was well-known for his group-theoretical insights. His lectures focused on the construction of spin eigenfunctions and the use of unitary group methods in configuration interaction (CI), essential for handling electron correlation efficiently.

### Prof. Osvaldo Goscinski

A key figure at Uppsala, Goscinski delivered incisive lectures on Green's function methods, electron correlation, and relativistic quantum chemistry, emphasizing their relevance to accurate electronic structure calculations.

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## Prof. Yngve Öhrn

Then at Uppsala (later at the University of Florida), Öhrn lectured on molecular collisions and time-dependent quantum mechanics. He demonstrated how propagator techniques capture many-body dynamics and underpin scattering theory.

## Prof. Herbert Jehle

A distinguished theoretical physicist from George Washington University, Jehle's lectures at Dalseter focused on **quantum biology,** where he explored the application of quantum principles to biological systems. His talks uniquely combined scientific depth with a philosophical perspective, offering a broader context to the Institute's themes.

## Rhythms of Uppsala: Where Science Met Sport

While the lectures at the Summer Institute were intellectually demanding and deeply enriching, the daily routine at Uppsala also reflected Professor Löwdin's holistic vision of learning—one that embraced physical activity, nature, and informal interaction as essential elements of the scientific life.

Each afternoon, after lunch, Professor Löwdin himself would enthusiastically invite both participants and lecturers to play soccer. His energy and openness erased all formal boundaries. Scientists from different countries and disciplines could be seen chasing the ball with equal zeal under the afternoon sun. It was as if quantum chemists, theoretical physicists, and biologists found a common "field"—literally—to bond and relax.

The daily soccer match became a beloved ritual, remembered not just for its playfulness but for the easy camaraderie it fostered. It gave younger participants a chance to connect with world-renowned faculty on equal footing (sometimes quite literally), and added a joyful rhythm to the academic schedule.


*Per-Olov Löwdin leading a soccer team including lecturers: (L-R) Osvaldo Goscinski, Sam Trickey, Piet Phariseau, Jean-Louis Calais, and Ruben Pauncz. (Credit: Michael Hehenberger)*

## Cultural Encounters in Stockholm: Science, History, and Heritage

Beyond the academic rigor of the Summer Institute, the organizers ensured that participants were also given a taste of Sweden's rich cultural and historical heritage. One of the most memorable excursions during our time in Sweden was a visit to the Stockholm Concert Hall, the iconic venue where the Nobel Prize ceremonies are held each year on December 10th. Standing in that grand and solemn hall—where some of the greatest scientific minds in history had received the world's most prestigious honour—was an emotional moment. It felt symbolic: a quiet reminder of the ideals of excellence, perseverance, and global recognition that every young researcher aspires toward. For many of us, it was not just a building, but a temple of inspiration.

Another unforgettable visit was to the Vasa Museum, where we saw the legendary Swedish warship Vasa. Built between 1626 and 1628, the warship tragically sank just 1,300 meters into her maiden voyage on 10 August 1628. For centuries, the wreck lay forgotten beneath the waters of Stockholm harbour until it was miraculously rediscovered in the late 1950s and raised in 1961, with much of its original structure preserved.

We were deeply moved by the story of the Vasa—its ambitious engineering, tragic fate, and eventual resurrection. Seeing the massive, ornately decorated hull—now housed in the remarkable Vasa Museum in the Royal National City Park—was like stepping into a portal through time. The ship's story, much like the unfolding story of science itself, spoke of human ambition, fallibility, loss, and redemption.


*Swedish Warship "WASA" – sank in 1628; raised in 1961. (Source: Printed Postcard; personal collection)*

These visits were not simply sightseeing—they were reflections on human achievement and humility, intertwined with the scientific and philosophical discussions we were immersed in during the Institute. They offered perspective: that while we explore the laws of nature, we also carry the responsibility of learning from history.

## Dalseter: Where Ideas Climbed Mountains

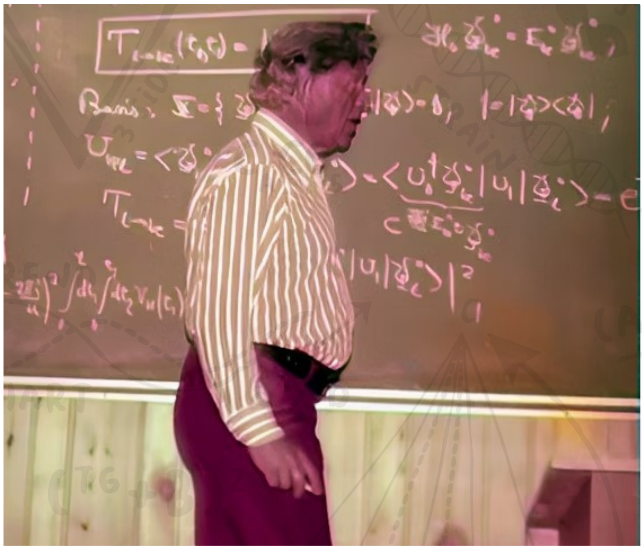
Our journey into Norway was smooth and scenic. Crossing the border by bus, we encountered no visa formalities—a relief that mirrored the serene Nordic landscape. Our destination was the picturesque Dalseter Høyfjellshotell, nestled high in the mountains.

Each morning, the lectures began sharp at 8:00 AM, in keeping with Professor Löwdin's unfailing punctuality. His sessions were followed by a series of enriching talks from other distinguished professors, running until around 4 PM, with a break for lunch. The academic atmosphere was intense, yet deeply stimulating.

At Dalseter, we were joined by the esteemed Professor Herbert Jehle, whose reflective lectures on quantum biology and the symmetry inherent in living systems added a philosophical depth to the program. His calm demeanour and profound insights left a lasting impression on many of us.

A particularly engaging session involved cultural presentations by the participants. Some spoke eloquently about their homelands, while others enhanced their talks with photographs or slide projections. It was a vibrant celebration of global diversity and scientific camaraderie.

Wednesdays were reserved for hiking in the surrounding mountains. Participants could borrow hiking kits, while others opted for leisurely walks to absorb the beauty of the local scenery—verdant trails, fresh alpine air, and panoramic views that seemed to mirror the heights of intellectual discourse we experienced indoors.


*Per-Olov Löwdin delivering a lecture in a Dalseter Hotel Lecture Hall. (Credit: RK Hosur)*

## Dr. Michael Hehenberger: A Lifelong Bond Forged in Science and Kindness

Among the treasured recollections from Dalseter, one remains especially vivid—an enduring symbol of warmth and quiet generosity. Acting on the advice of a mentor from home, I found myself needing a *portable typewriter* and a dependable *travel suitcase*. To my profound gratitude, Dr. Michael Hehenberger graciously offered to drive me to a distant shopping centre, ensuring I secured what I needed. That humble typewriter went on to serve me faithfully for nearly two decades, becoming an indispensable companion in my academic journey.

His act of kindness transcended mere professional courtesy. It reflected a rare spirit of empathy and human connection, leaving an imprint that I carry to this day.

To my great joy, nearly half a century later, I reconnected with him. In a gesture as generous as it was meaningful, he shared several heartfelt articles written in memory of Professor Per-Olov Löwdin, with whom he had been closely associated for ten years, affectionately referring to him as his *'lost father'*. I remain truly indebted to him for allowing me to include the evocative photographs he captured during the Summer Institute—images that now lend visual life to these recollections.

This story would remain incomplete without mentioning Dr. Hehenberger's personal impressions about Professor Löwdin (POL), under whose supervision he completed his Ph.D. at Uppsala University in 1975. In his article, *"Per-Olov Löwdin's Impact on a Lost Son"* published in *Advances in Quantum Chemistry, Volume 77, 2018,* Dr. Hehenberger has noted that:

- POL prepared his students for competitive life, both inside and outside academia.
- He trained them to present topics of great complexity succinctly, insisting: *"You must be able to explain something in 10 minutes—and do it convincingly."*
- He gave assignments and spent his valuable time checking their progress.
- He attracted first-rate scientists to his seminars and symposia.
- He encouraged students to be bold and tackle difficult problems, while reminding them that *"bread and butter"* work was also essential.
- He emphasized an *"economy of thinking",* valuing "fat symbols" and linear algebra for their conceptual power.

The profound influence of POL shaped Dr. Hehenberger's remarkable career trajectory. After completing his Ph.D., he spent two years (1975–77) at the University of Florida, first as a Postdoc and then as Visiting Associate Professor. Following research roles in materials science at Sandvik Hard Materials, Stockholm, he joined IBM Sweden in 1985, pioneering academic partnerships in computational chemistry, biology, structural engineering, computer networks, and supercomputing.

In 2000, IBM recognized Life Sciences and later Information-Based Medicine as strategic growth areas, with Dr. Hehenberger leading initiatives in these fields globally. His 23-year tenure at IBM took him to Paris (IBM Europe), California (Almaden Research, San Jose), and New York, where he led collaborations with academic and industrial life sciences organizations worldwide. He authored around 50 publications and book chapters, and his first book, *"Nanomedicine: Science, Business, and Impact,"* was published by Jenny Stanford Publishing in 2015.

Michael Hehenberger – Uppsala, Sweden (1975). (Credit: Michael Hehenberger)

After retiring from IBM in 2013, Dr. Hehenberger founded HM NanoMed LLC, a biotechnology company focused on advancing healthcare through nanotechnology, including writing, organizing conferences, and research in nanomedicine and genomics.

His remarkable achievements reveal the enduring influence of his most valued mentor, Professor Per-Olov Löwdin, whose guidance shaped his intellectual rigor, professional leadership, and unyielding commitment to advancing science for human benefit.

## The Summit of Dedication: Galdhøpiggen and Bygdin Lake

When in Norway, Professor Löwdin was not only teaching quantum chemistry but also leading mountain climbs. Michael assisted him in guiding Summer Institute participants to the summits of several mountains, including Galdhøpiggen, the highest peak in Scandinavia.

**Left Photo:** *Per-Olov Löwdin (POL) immersed in the group of students at the Galdhøpiggen Peak, Norway in the summer of 1975.*
**Upper Photo:** *POL posing alone at the Galdhøpiggen Peak.*
*(Credit: Michael Hehenberger)*

*Boat ride across the Lake Bygdin, Norway (Credit: RK Hosur)*

During the last phase of the Summer Institute, the most exciting and symbolic moment came when Professor Löwdin led a group of enthusiastic participants to climb the snow-clad peak of Galdhøpiggen. The mountaineering team had a long and challenging trip but ultimately reached the summit.

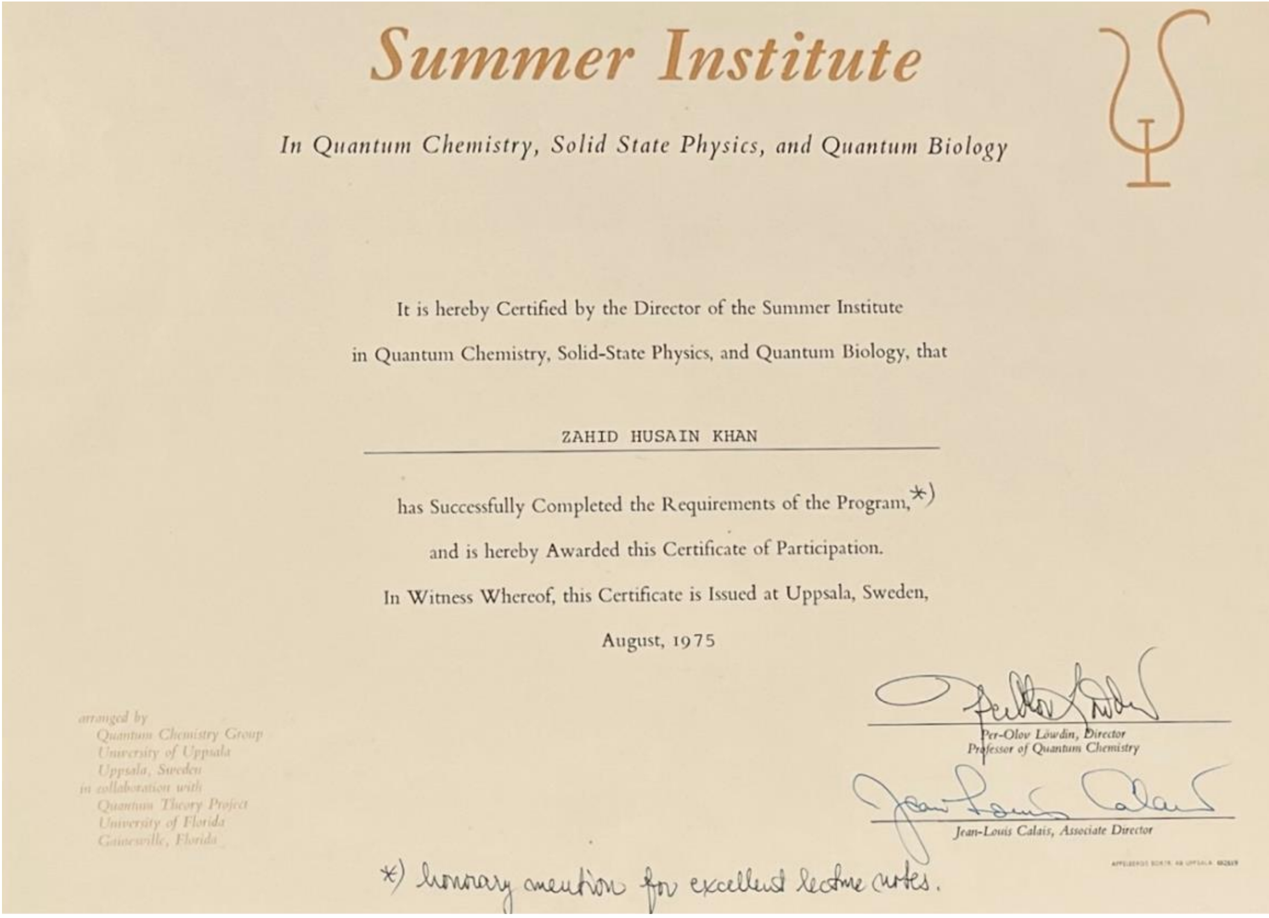
We learned the next morning that the entire team had returned to Dalseter Hotel after 2:00 AM. Incredibly, Professor Löwdin was in the lecture hall at 8:00 AM, as energetic as ever, ready to continue his teaching with undiminished dedication.

Others, myself included, chose a scenic boat ride across Lake Bygdin in Jotunheimen National Park—a tranquil experience amidst towering fjords. We took the last boat ride and reached the hotel in the evening.

## Farewell from Dalseter: A Lasting Souvenir

After spending three weeks at the Summer Institute in Dalseter, the final day arrived. On the evening of 31 August 1975, we boarded the bus to Oslo International Airport, each departing to their respective countries. Among the mementos of this journey, the souvenir presented by Dalseter Høyfjellshotell remains with me even after fifty years, forever refreshing the sweet memories of Norway's majestic beauty and the warm, friendly environment of the Summer Institute.


*Souvenir from Dalseter Høyfjellshotell*


Summer Institute

In Quantum Chemistry, Solid State Physics, and Quantum Biology

It is hereby Certified by the Director of the Summer Institute
in Quantum Chemistry, Solid-State Physics, and Quantum Biology, that

ZAHID HUSAIN KHAN

has Successfully Completed the Requirements of the Program,*)
and is hereby Awarded this Certificate of Participation.
In Witness Whereof, this Certificate is Issued at Uppsala, Sweden,
August, 1975

arranged by
Quantum Chemistry Group
University of Uppsala
Uppsala, Sweden
in collaboration with
Quantum Theory Project
University of Florida
Gainesville, Florida

Per-Olov Löwdin, Director
Professor of Quantum Chemistry

Jean-Louis Calais, Associate Director

*) honorary mention for excellent lecture notes.

## Legacy and Gratitude: A Tribute to Löwdin

Years later, I fulfilled a quiet dream—to publish in *The International Journal of Quantum Chemistry.* My 1992 research paper, ***"A Theoretical Study of Electronic Spectra of Radical Cations of Some Dihydroxynaphthalenes,"*** found its place there and published in its Vol. 42, pp. 1717–1735, after careful expansion of the theoretical section, in true spirit of the journal, following the comments of the editor.

Looking back, I now wish I had dedicated it to Professor Löwdin. But as 2025 marks the **International Year of Quantum Science and Technology,** I take this opportunity to posthumously dedicate that work to him, with gratitude and admiration.

The most cherished souvenir of that journey is my **Certificate of Participation,** signed by Prof. Löwdin himself—with a handwritten note: *"honorary mention for excellent lecture notes."*

It is a personal treasure, preserved for five decades.

## Epilogue: A Journey Etched in Time

As the world marks a century of quantum mechanics, I reflect on the Summer Institute of 1975 not merely as a scientific event, but as a defining chapter of my life. It shaped my intellectual perspective, sharpened my research aspirations, and broadened my global scientific connections.

To Professor Löwdin, whose visionary leadership made it all possible; to the distinguished faculty, for their illuminating insights; and to Dr. Hehenberger, for his enduring kindness—I extend my deepest gratitude. ◆

***Dr Zahid H Khan*** *is an advisor at the Zaheer Science Foundation in New Delhi and a former Professor of Physics at Jamia Millia Islamia, a Central University in New Delhi. He can be reached via email at zhkhan1948@yahoo.com*

VIGYAN 2047 Volume 2 No. 9 September 2025 Pages 20–23

# Per-Olov Löwdin

## Father of Quantum Chemistry

Zahid H Khan and Nakul Parashar

In the vast constellation of twentieth-century science, few stars shine as enduringly as **Per-Olov Löwdin,** a man whose vision transformed quantum chemistry from a theoretical curiosity into a rigorous, internationally respected discipline. A gifted physicist, a master teacher, a founder of institutions, and a weaver of international scientific kinship, Löwdin's life was marked by intellectual brilliance, scientific tenacity, and philosophical depth.

Born in **Uppsala, Sweden, on October 28, 1916,** Per-Olov Löwdin displayed early signs of academic genius. Even as a young student at Uppsala University, he was known for his remarkable mathematical abilities, quickly earning the attention of faculty and peers. His formal education blossomed under the guidance of theoretical physicist **Ivar Waller,** and in **1948,** Löwdin earned his Ph.D. with groundbreaking work on the cohesive energy and elastic constants of ionic crystals. What made this work so extraordinary was not just its technical brilliance but the sheer audacity of its execution—it was carried out before the invention of digital computers.

Instead of relying on machines, Löwdin enlisted an army of bright science students armed with electrically powered calculators and ingenious numerical algorithms. In this collaborative feat of mental computation, Löwdin demonstrated the power of **first-principles quantum mechanics** in understanding physical properties of matter—laying foundational stones for what would become the discipline of quantum chemistry.

*Per-Olov Löwdin*
*(28 October 1916 – 6 October 2000)*
*(Credit: Uppsala Quantum Chemistry Group)*

Following his doctoral work, Löwdin undertook **postdoctoral research with Wolfgang Pauli,** one of the founding fathers of quantum mechanics. He also spent formative time at **MIT** with **John C. Slater's Solid-State and Molecular Theory Group,** where he became immersed in the American scientific landscape. Despite offers abroad, Löwdin returned to Sweden, facing an uncertain academic future in a country where quantum chemistry had no formal recognition or institutional support.

But his return marked the beginning of a remarkable journey. With critical research funding from U.S. defense agencies, Löwdin established the **Uppsala Quantum Chemistry Group,** initially comprising a modest team of students and visiting researchers like **Harrison Shull, George Hall, Ruben Pauncz,** and **Roy McWeeny.** Together, they forged a research environment known for its intense intellectual exchange, characterized by Löwdin's legendary seminars. Despite quantum

*Wolfgang Pauli (credit: wikipedia)*

*(Credit: Taylor & Francis Online)*

chemistry lacking official standing at Uppsala University—thus unable to grant Ph.D. degrees—many students devoted themselves to the subject, drawn by Löwdin's charisma and deep insights.

In **1959,** Löwdin's transatlantic scientific life truly began when he accepted an invitation from the **University of Florida** to establish a theoretical research group in quantum chemistry. This venture would become the renowned **Quantum Theory Project (QTP),** a flourishing center for theoretical chemistry and physics that still thrives today. Around the same time, Löwdin was awarded a personal chair in Quantum Chemistry at Uppsala University—finally granting the subject academic legitimacy in Sweden. Thus began a life divided between continents: half a year in Uppsala, half in Gainesville, Florida, for over four decades.

Löwdin's scientific contributions were vast, ranging from the development of key theoretical tools to fundamental ideas that continue to guide research today. Concepts such as **"natural orbitals," "spin projection," "correlation energy," "Löwdin orthogonalization,"** and **"reduced density matrices"** are now part of the essential vocabulary of quantum chemistry and condensed matter physics. His work was marked by mathematical elegance, conceptual clarity, and a deep understanding of both the limitations and possibilities of quantum mechanics.

Yet Löwdin's legacy is not only etched into equations and theories—it is also inscribed in institutions, symposia, and the lives of scientists across generations. From **1958 to 1987,** he and his collaborators organized the legendary **Scandinavian Summer Schools in Quantum**

**Concepts such as "natural orbitals," "spin projection," "correlation energy," "Löwdin orthogonalization," and "reduced density matrices" are now part of the essential vocabulary of quantum chemistry and condensed matter physics.**

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**Chemistry and Solid-State Physics,** often held in remote mountain locales. These schools were known for their rigorous academic sessions and equally intense mountain hikes—many led by Löwdin himself. Participants fondly recall the unique combination of scientific intensity and alpine adventure, which often sparked not just research ideas, but lifelong friendships.

Parallel to these were the **Winter Institutes** held with the University of Florida team, eventually evolving into the globally celebrated **Sanibel Symposia**—named after the idyllic Gulf of Mexico island where the first 17 gatherings were held. These meetings brought together leading minds in physics and chemistry, fostering global scientific collaboration long before the internet made it commonplace.

In **1964,** Löwdin launched the influential book series *Advances in Quantum Chemistry,* and in **1967,** he founded the **International Journal of Quantum Chemistry,** serving as its first editor. These publishing platforms gave the field both structure and visibility, nurturing its growth into a respected scientific discipline. He was also instrumental in establishing the **Academy of Quantum Molecular Science in Menton,** further emphasizing his role as a builder of institutions and networks.

To walk into Löwdin's office in Gainesville or Uppsala was to witness a global web of influence: his wall map marked with colored pins showed where alumni of his groups now worked—on every continent and in almost every country. His students and collaborators became the next generation of leaders in quantum science, perpetuating his methods, style, and values.

Löwdin received numerous prestigious honors in his lifetime. He was a member of several national academies—including those of Sweden, Norway, Denmark, Finland, and Korea—as well as the American Philosophical Society, the American Chemical Society, and the American Physical Society. He was a **Chevalier of the Legion of Honor,** recipient of the **Lavoisier Medal** (Gold) from the French Academy of Sciences, and the **Oscar Carlson Medal** (Gold) from the Swedish Chemical Society. He also received the **Niels Bohr Medal** from WATOC in 1987.

*(Credit: Taylor & Francis Online)*

Despite his towering academic stature, those who knew Per-Olov Löwdin best remember a man of boundless **energy, enthusiasm, and curiosity.** He was passionate not only about science, but also about **music theory,** and was a skilled pianist. His philosophical musings on science, symmetry, and the meaning of knowledge often surfaced in lectures and conversations, adding an introspective dimension to his scientific persona.

He passed away on **October 6, 2000,** in his hometown of **Uppsala,** surrounded by his closest family. His passing marked the end of an era—but his spirit remains alive in the institutions he built, the ideas he championed, and the people he inspired.

To many across the world—students, colleagues, and fellow adventurers—**Per-Olov Löwdin** was not just a scientist. He was a **mentor, a visionary, a bridge-builder, and a friend.** His life's work exemplified the fusion of rigorous science with humanistic values. He didn't just transform quantum chemistry—he helped shape the global community that sustains it. ◆

***Dr Zahid H Khan** is an advisor at the Zaheer Science Foundation in New Delhi and a former Professor of Physics at Jamia Millia Islamia, a Central University in New Delhi. He can be reached via email at zhkhan1948@yahoo.com*

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# Quantum Chemistry

## Unveiling the Invisible World of Molecules

Amitesh Banerjee

At the intersection of physics and chemistry lies a field that probes the universe at its most fundamental level—**Quantum Chemistry.** Using the strange and powerful principles of quantum mechanics, quantum chemistry allows scientists to peer into the invisible world of electrons, orbitals, and atomic interactions. It enables the prediction of molecular behavior with remarkable precision and continues to revolutionize everything from drug discovery to materials science.

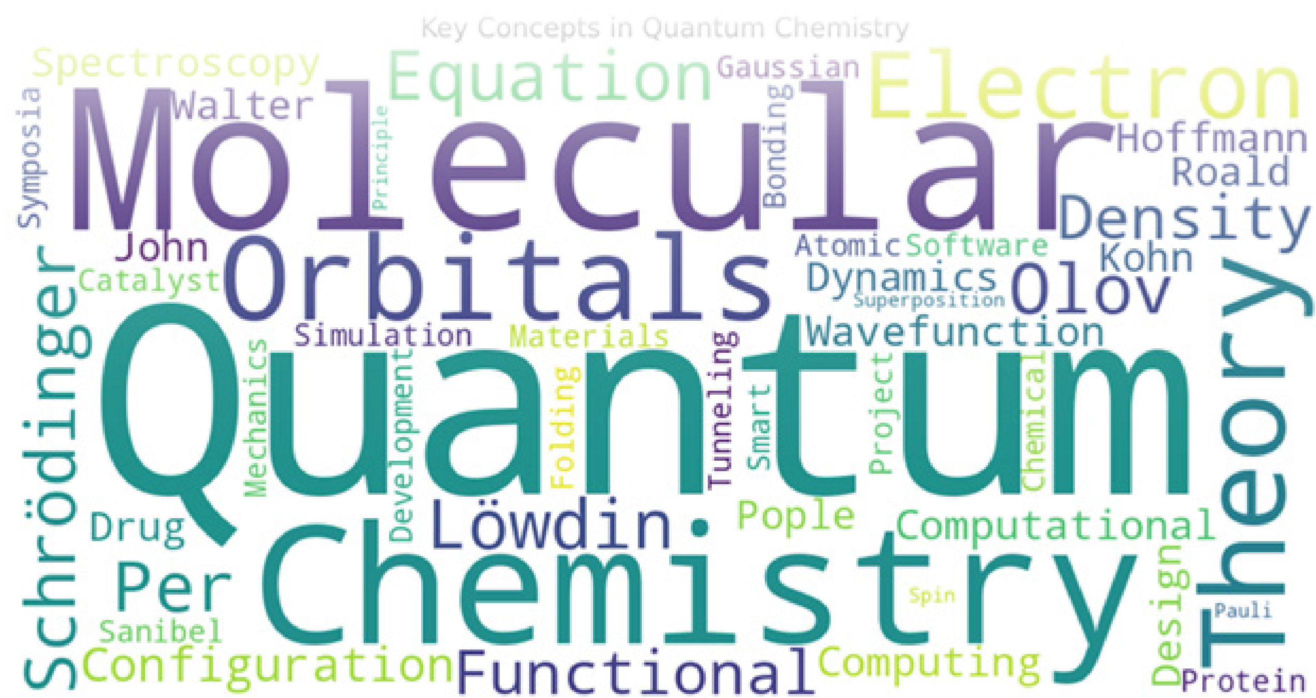
This is not just a story of numbers and equations. It's also a narrative of human brilliance, bold hypotheses, and communities of researchers who dared to model the molecular world before they could see it.

**Quantum chemistry** is the application of quantum mechanics to chemical systems. Unlike classical chemistry, which relies on macroscopic properties and approximate models, quantum chemistry deals with the behavior of **electrons and nuclei** at atomic and subatomic scales using exact or semi-exact mathematical formulations.

At its heart lies the **Schrödinger equation,** a complex differential equation that describes how the quantum state of a system changes over time. The solution to this equation—the **wavefunction (Ψ)**—gives us complete information about a molecule's energy, structure, and electron distribution.

Quantum chemistry treats electrons not as particles in neat orbits, but as wave-like entities described by probability clouds. These descriptions allow for detailed insights into **chemical bonding, reactivity, and molecular properties.**

The origins of quantum chemistry go back to the early 20th century, following the birth of quantum mechanics by pioneers like **Max Planck, Niels Bohr,** and **Erwin Schrödinger.** Their insights into atomic structure laid the foundation.



Key milestones include:

- **1926:** Schrödinger's equation explains the hydrogen atom — a landmark in theoretical chemistry.
- **1930s–50s:** Emergence of **molecular orbital theory** and **valence bond theory.**
- **1950s–70s:** Advent of digital computers revolutionizes the field, enabling approximate solutions to complex molecules.
- **1980s–2000s:** Rise of **Density Functional Theory (DFT)** and software like **GAUSSIAN** and **MOPAC.**
- **Present:** Integration with **quantum computing, machine learning,** and large-scale simulations.

## Key Concepts in Quantum Chemistry

| Concept | Description |
|---|---|
| **Wavefunction (Ψ)** | Describes the quantum state of electrons in a molecule |
| **Atomic & Molecular Orbitals** | Regions of space where electrons are likely to be found |
| **Electron Spin & Pauli Principle** | Dictates how electrons fill orbitals and affects magnetism |
| **Schrödinger Equation** | Central equation of quantum mechanics applied to atoms and molecules |
| **Ab initio Methods** | Calculations based only on physical laws (e.g., Hartree-Fock, MP2) |
| **Density Functional Theory (DFT)** | Focuses on electron density; popular for large-scale systems |
| **Quantum Tunneling** | Particles passing through barriers — critical in reactions and enzymes |

## 🧪 Real-World Applications of Quantum Chemistry

Though often viewed as a theoretical branch of science, **quantum chemistry** is far from being confined to blackboards and equations. In fact, it plays a pivotal role in shaping several modern technologies and scientific breakthroughs. By revealing the behavior of electrons and atoms at quantum scales, quantum chemistry enables us to design better drugs, engineer more efficient catalysts, develop advanced materials, and even explore life's fundamental processes.

Let's explore some of the most impactful domains where quantum chemistry is making a real-world difference.

### 💊 Drug Design & Pharmaceuticals

One of the most transformative applications of quantum chemistry lies in **pharmaceutical research.** Using computational quantum models, scientists can predict how a potential drug molecule will interact with its biological target—typically a protein or enzyme. This predictive power significantly shortens the trial-and-error phase of drug discovery, reducing costs and accelerating development timelines.

By simulating **molecular interactions** before synthesis, quantum chemistry helps researchers fine-tune the structure and reactivity of drug candidates, leading to **safer and more effective medicines.**

### ⚗️ Catalysis & Green Chemistry

Catalysts are substances that speed up chemical reactions without being consumed. Designing **efficient, selective, and sustainable catalysts** is essential for industries ranging from fuel production to food processing.

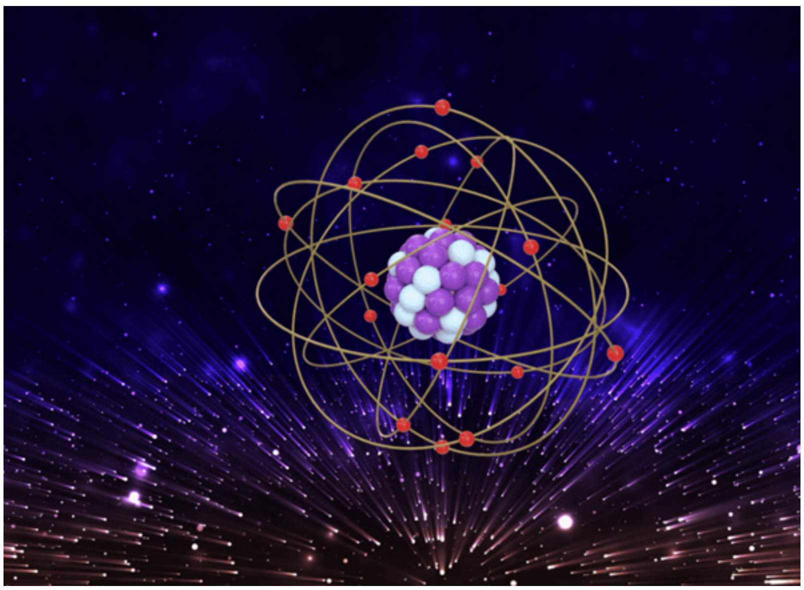
Quantum chemistry provides insight into **reaction pathways** at the atomic level, allowing chemists to identify where energy barriers lie and how to minimize them. This has a profound impact on **green chemistry,** where the goal is to develop industrial processes that are not only efficient but also environmentally friendly.

Through these simulations, quantum chemistry is guiding the development of **cleaner, safer, and more sustainable catalytic systems.**

## Materials Science & Nanotechnology

From ultra-thin **graphene** sheets to advanced **battery materials** and **quantum dots,** quantum chemistry is at the heart of materials innovation. It allows scientists to model how **atomic and molecular structures** affect electrical, thermal, and mechanical properties.

Quantum simulations can predict how materials will behave under stress, how electrons move through semiconductors, or how light is absorbed by solar panels. This predictive capability is invaluable in designing the next generation of **semiconductors, solar cells, smart textiles, and energy storage devices.**



## Spectroscopy & Light Interaction

Understanding how molecules interact with light is essential in **analytical chemistry.** Quantum chemistry helps explain how electrons transition between energy levels, providing the foundation for interpreting **absorption and emission spectra.**

This knowledge supports widely-used technologies like **NMR (Nuclear Magnetic Resonance), IR (Infrared), UV-Vis, and X-ray spectroscopy,** enabling chemists to determine the structure and composition of unknown substances with precision.

## Quantum Biology

Quantum chemistry has also found fascinating applications in biology. By modeling **photosynthesis, enzyme mechanisms,** and **protein folding,** researchers are uncovering **quantum phenomena in living organisms.** For instance, quantum tunneling may play a role in enzymatic reactions, and quantum coherence might enhance energy transfer in photosynthetic systems.

This growing field of quantum biology bridges the gap between physics, chemistry, and life sciences, opening new avenues for inter-disciplinary research. In short, quantum chemistry is not just a theory—it is an indispensable **toolbox for solving real-world problems,** shaping the future of science and technology one molecule at a time. Solving quantum equations for real molecules requires immense computational power. Thanks to advances in computer science, chemists now routinely use simulation tools to model molecules of hundreds of atoms.

Popular software:

- **Gaussian** – General-purpose electronic structure modeling
- **ORCA, VASP, NWChem, TURBOMOLE –** Specialized for various calculations

Emerging frontiers include:

- **Machine Learning-Accelerated Quantum Chemistry**
- **Quantum Algorithms** on **quantum computers** (e.g., Variational Quantum Eigensolver)
- **Cloud-based Simulations** for real-time molecule analysis

Beneath all the code and computation lies a very human story—one of **brilliant minds** who laid the foundations of quantum chemistry through vision, courage, and collaboration.

## Per-Olov Löwdin: Architect of a Discipline

Often credited as the **father of quantum chemistry,** Löwdin brought structure to the field by founding the **Quantum Theory Project** in Florida and the **International Journal of Quantum Chemistry.** His summer schools in Scandinavia and **Sanibel Symposia** fostered global scientific exchange.

## John Pople & Walter Kohn: The Mathematical Pioneers

Pople's work on computational models made **ab initio methods** accessible to chemists worldwide. Kohn's **Density Functional Theory** became the bedrock of modern molecular simulations.

## Roald Hoffmann: The Theoretical Chemist

His contributions to **frontier molecular orbital theory** bridged theoretical chemistry with practical insights, explaining how and why reactions occur.

These thinkers didn't just advance knowledge—they created **communities.** Through schools, symposia, and journals, they nurtured a culture of **open inquiry, mentorship,** and **global collaboration** that lives on today.

Quantum chemistry stands on the brink of yet another revolution—one powered by **quantum computing.** These next-generation machines operate on **qubits,** enabling parallelism far beyond classical computing.

Potential breakthroughs include:

- Modeling **large biomolecules** with unprecedented accuracy
- Solving **intractable electronic structure problems**
- Discovering **new materials** for energy, sustainability, and space

With collaborations between chemists, physicists, computer scientists, and AI experts, the future of quantum chemistry is not just bright—it's **exponentially powerful.**

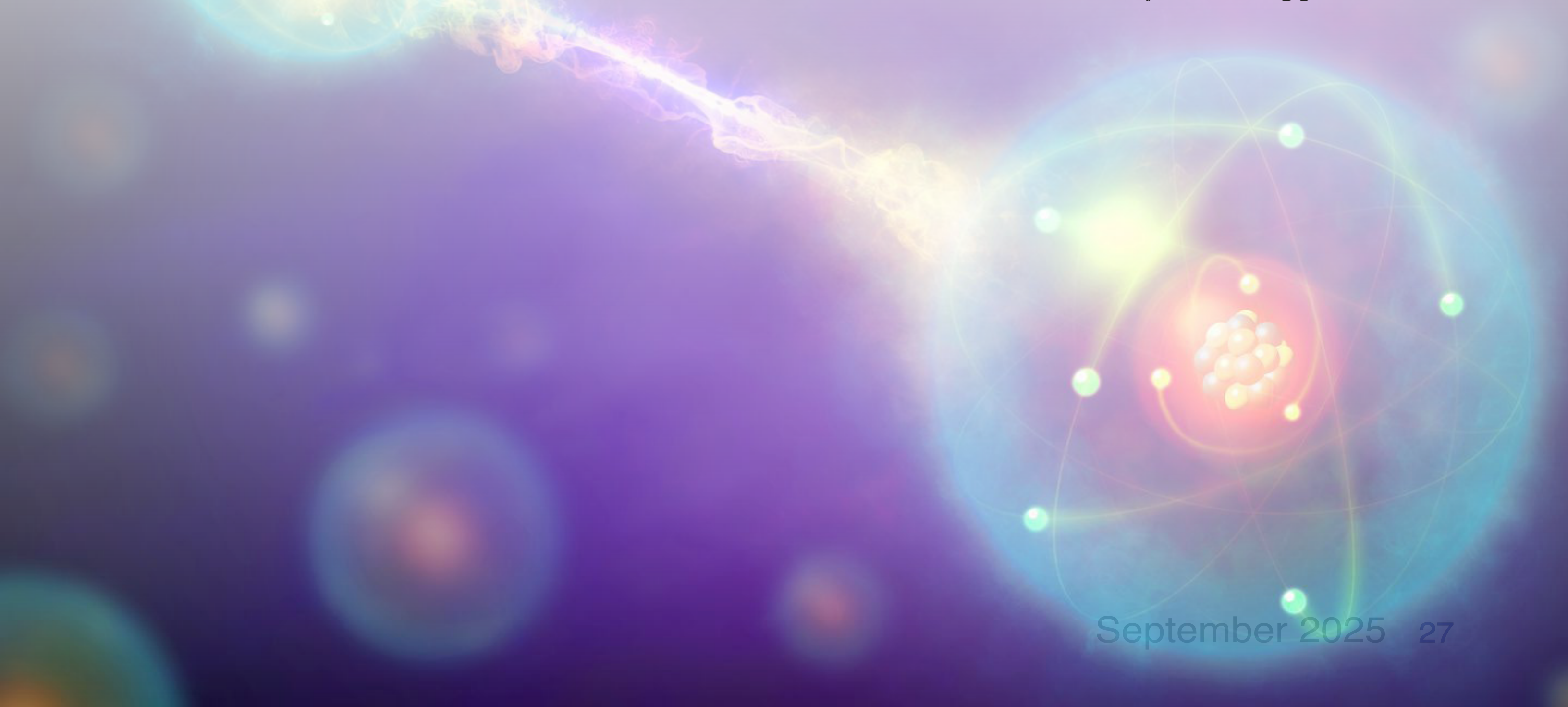
Quantum chemistry gives us a language to describe the indescribable—the bonds we cannot see, the reactions we cannot touch, and the forces that hold matter together.

It transforms chemistry from an experimental art into a **predictive science,** where **theory guides synthesis,** and where **simulations shape reality.**

In an era defined by **molecular challenges**—from climate change to medicine to energy—quantum chemistry equips us with the tools to think at the smallest scales and act at the largest.

It reminds us that within the mysterious dance of electrons and the elegance of a wavefunction lies the key to solving some of humanity's greatest problems. ◆

***Sh. Amitesh Banerjee*** *is a science communicator. He can be reached via email at amitesh.shantifoundation@gmail.com*



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# Tribology of Prime Movers: IC Engine

## Kamal Mukherjee

Basically, the function of a prime mover is to convert the input energy into a useful work. Thus, all types of engines & electric motors are known as a prime mover & used to get the useful work by utilising the input energy. The engine convert heat into work by expansion or increase in volume of a working fluid into which heat is introduced by combustion of a fuel either external to the engine as in a steam engine or internally by the burning of a combustible mixture in the engine itself known as 'internal combustion engine' (ICE) or a jet engine. For easier understanding of the engine tribology aspects, an automobile engine is selected here as the prime mover.

The reciprocating internal combustion engine are popular, reliable & versatile with a large range of power units available in both petrol and diesel engines as applicable to bike, scooter, car, jeep, van. truck, tractor, bus, mid to light duty trailers, off highway trucks, train, boat, ship, agriculture-domestic pumping, construction & mining vehicles & machinery etc. as per their needs. LPG & CNG engines are in automobile operations. Hydrogen engines are now used on trial basis.

The largest number of ICE are used in cars, jeeps (SUVs), light & heavy-duty vehicles world over among the others. Thus, a typical case of petrol engine is referred here. The data collected from various published studies on the energy distribution are shown as an average values applicable for petrol cars worldwide. Typical distribution of the mechanical friction losses ~78% in a petrol engine car are as shown in Fig-1 (ref. Pinkus & Wilcock, lang, Anderson, Bartz, Taylor, Hikita, Holmberg et al-2012).On the other hand, typical fuel energy dissipation of ~ 74% in a Petrol car is shown in Fig-2.

With the new technology & tribology in passenger cars, friction losses could be reduced by 18% in the short term (5–10 years) as per Holmberg et al. This would equal worldwide economic savings of 174,000 million euros; fuel savings of 117,000 million litres and $CO_2$ emission reduction of 290 million.

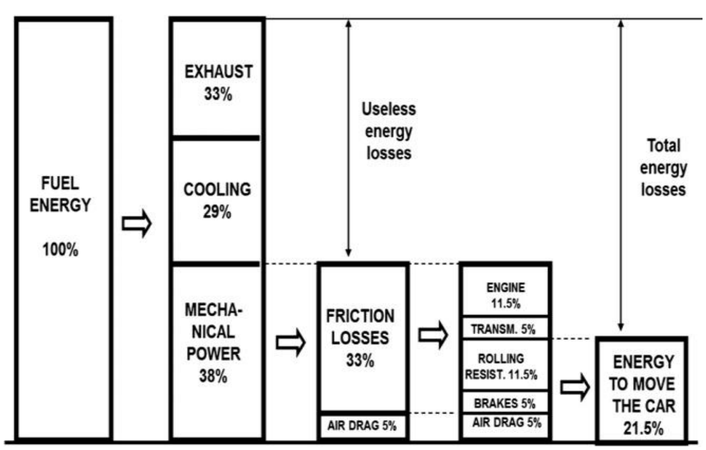


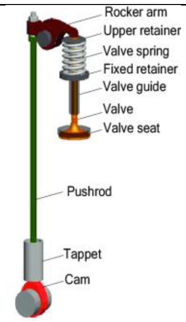

Fig.-1: Distribution of energy in a typical passenger Petrol carr

| Energy Input | Energy Loss | % Loss |
|---|---|---|
| Fuel (Potential Energy) | Exhaust | 33% |
| | Cooling | 29% |
| | Engine Friction | 12% |

| Conversion to: |
|---|
| 1.Kinetic Energy: Motion |
| 2.Thermal Energy: Heat loss |
| 3.Fuel potential energy reduction |

Fig-2: Typical fuel energy dissipation in a Petrol car

### Table-1: Main engine components subjected to friction & wear

<table>
<tr><th>Piston & Rings</th><th>Cylinder (Liner)</th><th>Cam Shaft</th><th>Valve Train</th></tr>
<tr><td></td><td></td><td></td><td>
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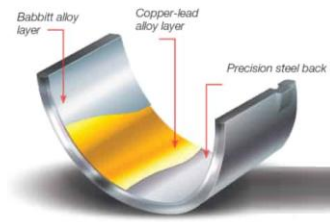
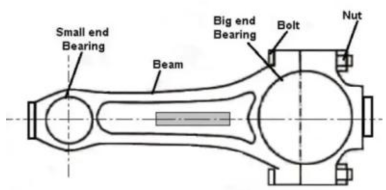
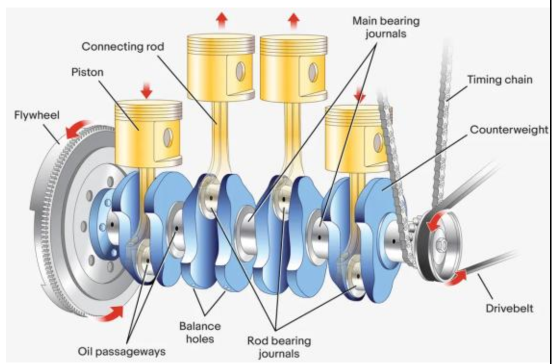
<tr><td colspan="2">Engine bearings</td><td colspan="2">Insidious components of engine</td></tr>
<tr><td colspan="2">

Connecting Rod

</td><td colspan="2">
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**Impact of friction:** The main frictional losses in an engine are due to friction between the piston with the cylinder walls, friction in various bearings, camshaft, crankshaft, valve train as shown in table-1 and also the energy spent in operating the auxiliary equipment such as cooling water pump, ignition system, fuel pump, fan, alternator etc.

**The Piston Ring Assembly (PRA) Friction:** PRA friction may best be characterized by the simple reciprocating motion of the piston within the liner, leading to areas of mixed and boundary lubrication at top and bottom dead centre followed by the regions of lubrication in between as shown in table-2. Due to combustion the pressure inside the cylinder increases which promotes higher friction. The tribological studies of the piston ring friction zone, viscous shear which incorporate mixed lubrication conditions & wide variation with a host of influential parameters like temperature etc.

**VALVE TRAIN FRICTION:** The valve train friction occurs in the cam/follower interface, cam bearings/ seals, rocker arm, pivots, and tappets. The cam interface, tappet and bore friction account for the majority of friction. The valve train frictional losses typically account for 7% to 15% of the total mechanical losses of engine. In heavy-duty engines, the valves are usually operated by means of push-rods and rockers that receive their motion from a crankcase mounted camshaft.

**ENGINE BEARING FRICTION:** Different components of engine causes bearing frictions e.g. the crankshaft main bearings, connecting rod big-end & small-end bearings, camshaft bearings, and rocker arm bearings. High loadings in these bearings can be supported along with low friction due to complete separation of moving parts by a thick lubricant film. Engine bearings account for 20 to 30% of the total engine frictional losses. The highly stressed bearings in the engine are in the connecting rod big-end/small-end bearings and the crankshaft main bearings.

### Table-2: Engine Friction Energy Loss Distribution

| | Hydrodynamic Lubrication (HDL) | Elasto-Hydrodynamic-sliding contact Lubrication (EHDS) | Mixed Lubrication (ML) | Boundary Lubrication (BL) |
|---|---|---|---|---|
| **Petrol Car** | 40 % | 40 % | 10 % | 10 % |

**Table-3: Engine Friction Energy Loss Distribution in its main components**

| Engines used in | Piston assembly | Bearings and Seals (HD) | Valve Train (ML) | Pumping and Hydraulics Viscous Losses (VL) |
|---|---|---|---|---|
| **Passenger Cars** | 45% (45–55%) | 30% (20–40%) | 15% (7–15%) | 10% |

**ENGINE AUXILIARY POWER LOSSES:** Engine auxiliary power losses come from built-in accessories such as coolant pumps, oil pumps and fuel injection pumps, fans, alternators, air conditioning, and power-steering pumps.

**FUNCTIONSOFENGINELUBRICATING OIL:** Lubrication is an ancient art and modern science. In ICEs, high shear rates and high stress are generated in bearings and liner-piston-ring zones. Lubricants for engines need to fulfil several important functions in addition to the best known – controlling friction and wear to protect the engine against rusting, cooling & sealing the piston-ring-liner surfaces, against leakage of the combustion gases & cleaning by minimizing deleterious effects of combustion products etc. The lubricant has to perform these functions for periods of hundreds of hours between oil changes, under a wide variety of climatic and operating conditions. In today's trend of high power to weight ratio engines of compact size deliver high power, causes extreme thermal stressing and oxidation of the engine oil. The oil must remain fluid under all these conditions to perform its functions, ideally maintaining the right physical properties to perform them efficiently. Premium quality engine oil is formulated with a top-quality base oil with advanced technology-based additives in order to protect the automotive engine. ICE oils are graded based on the Society of Automotive (SAE) standard, which groups oils according to their viscosity.

**Impact of temperature on the engine:** ICEs are an interesting illustration of variation in temperatures in a machine and the corresponding times of exposure of the lubricants to those temperatures. There have been dramatic improvements in the life of engine oils in the past 70 years. In a typical passenger car, the engine oil change period was at 1500 Km in 1949, but this increased to 10,000 Km by 1972 and about 15,000 Km by 1998 owing to the use of synthetic oils. The general trend to higher specific power leads to higher operating temperatures. Different lubrication zones in the engine components are- 1) Engine bearings and seals mainly operate under hydrodynamic lubrication (HD), 2) The valve train operates under mixed lubrication (ML), which combines: a) Hydrodynamic lubrication (HD), b) Elastohydrodynamic lubrication (EHD) & c) Boundary lubrication (BL). The most critical is boundary lubrication zone, where the oil film is so less & thin that ultimately the resultant rough surfaces make frequent contacts that leads to higher friction. Based on various sources, the engine friction energy loss distribution as shown in table-3.

## Tribology Solutions

Smart & energy efficient oils: Nowadays the trend is to use low viscosity oils like 5W-30, 5W-20, 02W-20 etc. in place of 20W-40, 15W-40 viscometrics engine oils used previously. Thus, the high temperature high shear viscosity of the gasoline engine oils is reducing to 2.6 cSt.- 2.9 cSt. as against in the past of 3.7 cSt. Advantage of using low viscosity oil actually reduces the viscous drag thus it lowers the fluid friction that gives better fuel economy.

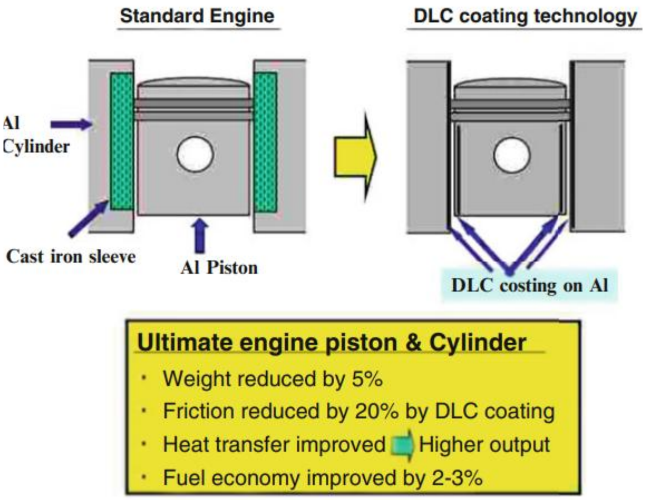


**Fig-3: DLC coated aluminium alloy piston & cylinder for ultra-low friction engine**

Different types of special additives e.g. Anti Wear (AW), Extreme Pressure (EP) & Friction Modifier (FM) are added in the lubricating oil. The addition of friction modifier additives like glycerol mono-oleate (GMO) to a polyalphaolefin (PAO) oil gave a friction coefficient of 0.05 in sliding contact. Of late, the use of certain nanomaterials as anti-friction and anti-wear additives has given very promising results. Customised oils are designed for the specific use of railroad engines, marine engines etc.

Low friction coatings for engine components: During the past two decades, research on low-friction materials and coatings has intensified, mainly because the traditional solid and liquid lubrication approaches would not alone meet the increasingly more stringent operational conditions of modern mechanical systems, including engines. A tribometer test indicated that significant reduction in hydrodynamic friction is achieved by applying textures (creating dimples on its surfaces) on cylinder liner surfaces & also on the piston skirts. The resultant friction is further reduced by using different oil additives along with low-friction DLC coatings as shown in Fig-3.

Smart metals: the connecting rods & valve train components made from titanium alloys are used in racing car engines to reduce the reciprocating weight without compromising the strength. Insulation of combustion chamber by

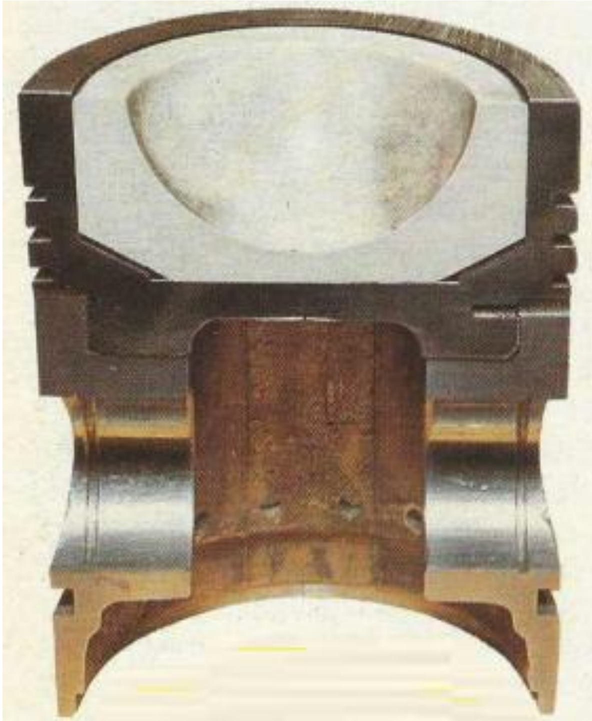

**Fig-4: Ceramics used as inserts in piston crowns**

ceramics, as inserts are applied to reduce the heat loss to gain the thermal efficiency & also to reduce the required radiator capacity, Fig-4. Ceramic turbocharger rotors exploit their lower material density & hence reduced inertia by showing reduced response time. Insulation of exhaust ports to reduce the heat rejection to coolant & improve the turbocharger efficiency by increasing the temperature of the exhaust gases. ◆

***Kamal Mukherjee**, a prolific science writer and nutritionist, is an active member of the Tribological Society of India and has held executive leadership roles in major national organizations. He can be contacted at kamalcbm28@gmail.com.*

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# When Nerves Fail

## Courage of Mrs. Manju Dutta

A.K. Gupta

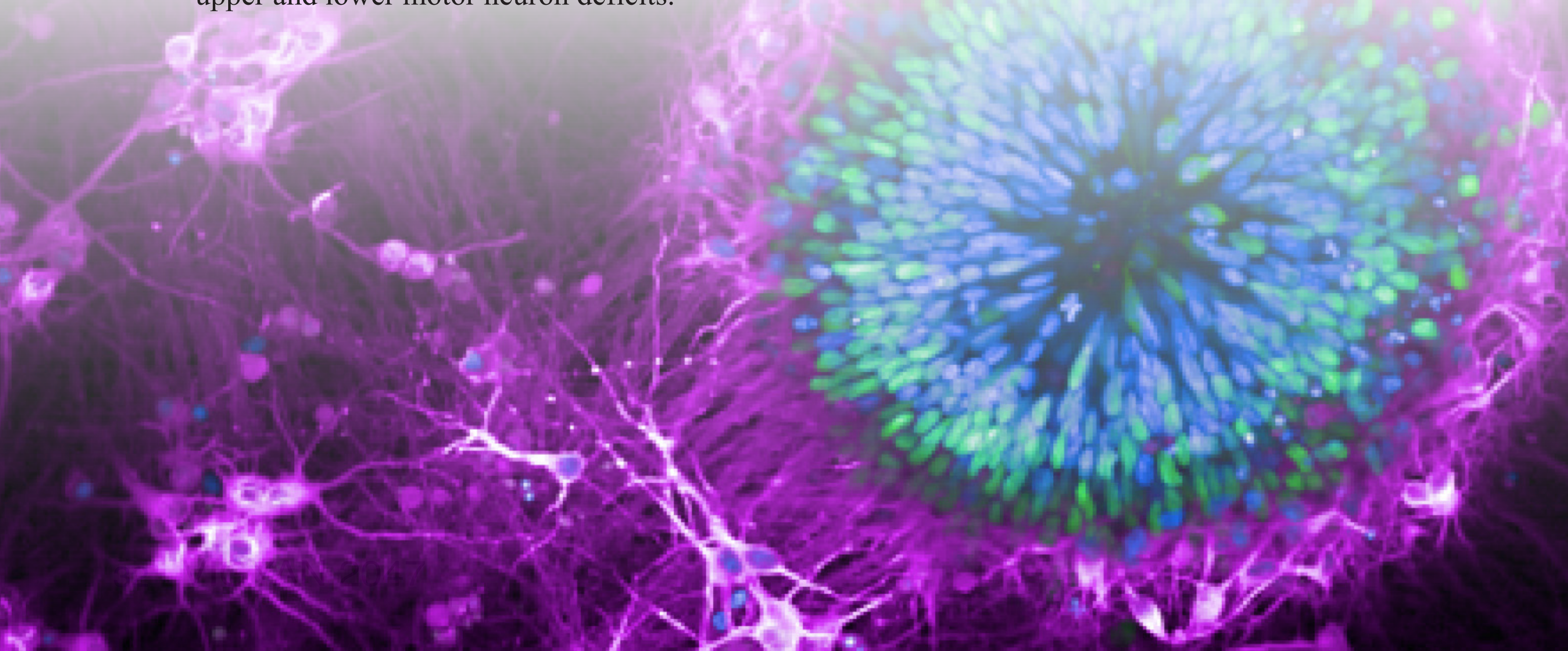
There are few illnesses that inspire as much fear and helplessness as Motor Neuron Disease (MND). Unlike infections or injuries that arrive suddenly, MND creeps in silently, manifesting as a weakness here, a stumble there, or a slurred word that refuses to clear. Over months and years, it grows into a condition that relentlessly strips away independence—stealing the ability to walk, speak, swallow, and ultimately even breathe—while the mind remains intact, painfully aware of every decline.

Motor Neuron Disease is not a single entity but a group of degenerative disorders that share a common feature: the progressive loss of motor neurons, the nerve cells responsible for controlling muscles. Without these vital messengers, muscles weaken, waste, and eventually fail. Unlike sensory nerves, which allow us to feel heat, pain, or touch, motor neurons are purely about movement. Their breakdown explains why patients with MND often retain sensation but lose control over their own bodies.

Globally, the most well-known variant of MND is Amyotrophic Lateral Sclerosis (ALS), popularized through the stories of physicist Stephen Hawking, who defied its prognosis by living for decades, and baseball player Lou Gehrig, whose name became synonymous with the disease in the United States. For most patients, however, the prognosis is far less forgiving.

Clinicians classify MND into several subtypes, depending on whether upper motor neurons (from brain to spinal cord) or lower motor neurons (from spinal cord to muscles) are more affected:

- **Progressive Bulbar Palsy:** Speech and swallowing are most severely affected. Patients choke easily and may lose their voice.
- **Pseudobulbar Palsy:** Emotional instability, bursts of uncontrollable laughing or crying, and spastic tongue movements are typical.
- **Progressive Spinal Muscular Atrophy:** Begins with weakness and wasting in the limbs.
- **Primary Lateral Sclerosis:** Rare, affects upper motor neurons alone, leading to stiffness and spasticity.
- **Amyotrophic Lateral Sclerosis (ALS):** The most common and aggressive form, combining both upper and lower motor neuron deficits.



The course is almost always progressive. Median survival is 3–5 years from symptom onset in ALS, though milder variants may allow longer survival.

In Allopathy (Conventional Medicine), modern neurology has long struggled to halt MND. Today, only a handful of drugs are approved worldwide. Riluzole, introduced in the 1990s, reduces glutamate toxicity in neurons and can extend survival modestly. Edaravone, an antioxidant, slows functional decline in some patients. Yet these are not cures, and the disease still progresses.

In parallel, homeopathy has approached MND with a focus on individualized treatment, looking not just at physical symptoms but also the patient's personality, fears, and emotional state. Remedies such as Plumbum Met. for paralysis and emaciation, Rhus Tox for stiffness, Causticum for speech and swallowing issues, Phosphorus for weakness, and Lachesis for choking and emotional lability have all been used. While critics debate the mechanisms, patients often report symptomatic relief, slower progression, and improved quality of life, which are invaluable in diseases with limited conventional options.

Ayurveda emphasizes strengthening the nervous system through a combination of Rasayana therapy (rejuvenation), Panchakarma detoxification, herbal medicines such as Ashwagandha and Brahmi, and dietary regulation. Yoga and pranayama are recommended to maintain breathing function and emotional balance.

Supportive Therapies: Across systems, physiotherapy, occupational therapy, speech therapy, counseling, and nutritional support are indispensable. Assistive devices — walkers, braces, speech boards—extend independence. Emotional support groups also play a vital role, both for patients and caregivers.

## A Patient's Journey
## *Case Study of Mrs. Manju Dutta*

Amidst these medical details, it is the personal stories that bring MND to life. One such story is that of Mrs. Manju Dutta, a 55-year-old woman from Bhubaneswar, Odisha, who bravely fought the disease between 2005 and 2008 under the care of Prof. Dr. A.K. Gupta, MD (Hom.)

Her ordeal began shortly after a hysterectomy in 2003. She noticed weakness in her left hand and difficulty straightening her fingers. Soon, her legs weakened, and by 2005, she had frequent backward falls, imbalance, and slurred speech. Eating became hazardous; she choked while swallowing and felt a persistent "sand-like" irritation on her tongue.

By the time she presented her case online in October 2005—later followed up in person in January 2006—she was already unable to walk without support, her arms raised only to chest level, her tongue trembling, and her hands and legs visibly emaciated.

What made Mrs. Dutta's case deeply human was not just her physical suffering but her emotional vulnerability. She was terrified of being alone, frightened of darkness and thunderstorms, and frequently wept. Her sleep was disturbed by dreams of snakes, fire, and dead relatives. Once a commanding personality, she now wrestled with inferiority, pessimism, and the haunting belief that her disease was incurable. She had long harbored an ambition to become a writer—an ambition cruelly cut short by illness.

Yet, within these vulnerabilities lay resilience. She enjoyed company, loved the seaside, was sympathetic to others, and often laughed even amidst tears.

Her progress was tracked meticulously through follow-ups:

- **March 2006:** No more falling backwards, reduced choking, better tongue sensation.
- **June 2006:** Speech slightly improved, no further deterioration.
- **2007:** Emotional balance improved, sleep steadier, cough reduced, and mobility marginally better with support.
- **2008:** Voice weakened again, profound weakness returned, and new burning sensations emerged.

Despite the disease's natural progression, she experienced long stretches of stability—remarkable in a condition that typically advances rapidly.

In early 2008, after nearly three years of resilience, Mrs. Dutta's condition worsened. Her

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speech grew faint, she felt burning sensations across her body, and her weakness became overwhelming. Finally, in March 2008, she passed away suddenly due to cardiac arrest.

Her death was a tragedy, but her journey remains a testament: through integrative care, emotional support, and sheer willpower, she managed to live more meaningfully with MND than the prognosis usually allows.

Mrs. Dutta's story is not isolated. Across India and the world, thousands of patients live with MND—many undiagnosed, many untreated, and most struggling in silence.

Her journey illustrates several lessons:

- **MND is more than a physical disease:** It attacks identity, ambitions, and confidence as much as it does muscles.
- **Holistic care matters:** Whether through homeopathy, Ayurveda, physiotherapy, or counseling, every supportive intervention buys dignity and comfort.
- **Caregivers play a vital role:** Mrs. Dutta's son, who first reported her case, was a pillar of strength—as many family members are in such conditions.
- **Research and awareness are urgent needs:** With limited conventional treatments, India and the world must invest more in both scientific research and supportive care networks. Motor Neuron Disease remains one of the unsolved mysteries of medicine. While science works towards finding cures, stories like that of Mrs. Manju Dutta remind us that patients need more than medicines—they need empathy, attention, and holistic care.

Every therapy that slows decline, every intervention that reduces choking or restores sleep, every moment of emotional reassurance matters. For a disease with no cure, quality of life is the true measure of success.

Mrs. Dutta's courage, her family's support, and her doctor's persistence stand as a beacon for all those grappling with MND. While her life ended abruptly, her journey continues to inspire—reminding us that when nerves fail, it is the spirit that must carry on. ◆

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# Celebrating the September Born Scientists

Bhupati Chakrabarti

These luminaries, born in the month of September, have each illuminated the path of human progress in their own right. Their discoveries have transcended the bounds of their respective fields, shaping the world as we know it. As we reflect on their lives and legacies, we are reminded of the boundless potential of the human spirit to inquire, innovate, and inspire. Through their work, these scientists have left an enduring legacy, a testament to the power of curiosity and the relentless pursuit of knowledge.

**Irene Curie,** the eldest daughter of the famous scientific couple Pierre Curie and Marie Curie, was born on September 12, 1897. She was a French chemist, physicist, and politician, and the wife of scientist Frédéric Joliot Curie. Irene Curie and her husband Frederic began their research on the study of atomic nuclei in 1928. They used gamma rays to detect positrons. In 1933, Irene and her husband determined the exact mass of the first neutron. When they exposed aluminum to alpha rays, they discovered that only protons could be detected. Based on the detectable electron and positron pairs, they proposed that protons decay into neutrons and positrons. In 1934 they were able to produce radioactive nitrogen from boron, radioactive isotopes of phosphorus from aluminum, and magnesium from silicon. A temporary radioactive isotope of phosphorus is produced by bombarding the naturally stable isotope of aluminum with alpha particles (i.e. helium nuclei). This led to an increase in the use of radioactive substances in medicine, and this discovery made it possible to produce radioactive substances that could cure diseases quickly, cheaply, and in large quantities. For this groundbreaking discovery, she jointly won the Nobel Prize in Chemistry in 1935, along with Irene and her husband. In 1956, Irene Curie was admitted to the Curie Hospital in Paris with leukemia, where she died on March 17 at the age of 58. The fatal illness was probably caused by radiation from polonium-210.

Of all the Danish scientists we know, perhaps the oldest is **Ole Romer**. A contemporary of Newton, Romer was born on September 19, 1644, two years after Newton. The great sci-entist Galileo had experimented with whether the speed of light was infinite. No definite direction was found from there. Romer assumed that the speed of light, although very high, was not infinite and he took the help of a natural phenomenon to measure that high speed. The speed of light he determined from Earth-based observations of an eclipse of Io, one of Jupiter's large moons, was about two-thirds of its current value. Although this value of the speed of light is slightly lower than the actual value, this experiment was the first definitive proof that the speed of light is not infinite. Another of Romer's works has a special connec-tion with the thermometer used to measure temperature. In fact, Romer invented a tem-perature scale at about the same time as German engineer John Gabriel Fahrenheit. This scale, known as the Romer scale, had the freezing point at 7.5 degrees (Romer) and the boiling point of water at 60 degrees (Romer). This temperature scale, introduced in 1701, was the first graduated temperature scale. Newton had previously proposed a temperature scale, but it did not have graduations and did not use the word temperature.

**Wilhelm Friedrich Ostwald** was born on 2 September 1853 and was a Baltic German chemist and philosopher,recognized as a founder of physical chemistry alongside van 't Hoff, Arrhenius, and Nernst. He won the 1909 Nobel Prize in Chemistry for work on catalysis, chemical equilibria, and reaction rates. Ostwald began his career at the University of Dorpat and later taught at Riga Polytechnicum and Leipzig University. He mentored future Nobel Laureates and declined Albert Einstein's early job application, though he later nominated him for the Nobel Prize. Ostwald developed the Ostwald Process for manufacturing nitric acid, crucial in fertilizer and explosives production. He introduced Ostwald's Dilution Law and clarified chemical catalysis. His work on polymorphism led to Ostwald's Rule and the concept of Ostwald Ripening, explaining changes in crystal forms over time. He also contributed to the Ostwald-Freundlich equation, describing solubility's dependence on particle size. After retiring in 1906, he turned to philosophy, art, and politics, publishing over 500 scientific papers and 45 books.

**Sir Mokshagundam Visvesvaraya** often referred to as MV, was born 15 September 1861 and was a distinguished Indian civil engineer, administrator, and statesman. He served as the 19th Dewan of Mysore from 1912 to 1918 and is celebrated as one of India's greatest engineers. His birthday is observed as Engineer's Day in India, Sri Lanka, and Tanzania. He was knighted KCIE by the British and awarded the Bharat Ratna in 1955 by the Indian government. Visvesvaraya began his engineering career in the Bombay Presidency and later worked on major irrigation and flood protection projects, including in Hyderabad and Visakhapatnam. He invented automatic weir floodgates, first used at Khadakvasla Dam, and later implemented at the KRS Dam in Mysore. As Dewan, he modernized Mysore by establishing key industries, banks, and educational institutions, including the Mysore Iron & Steel Works and Government Engineering College (now UVCE). Even in his 90s, he advised on major infrastructure like the Mokama Bridge over the Ganga.

**Asima Chatterjee** was born on 23 September 1917 and was a pioneering Indian organic chemist known for her contributions to organic chemistry and phytomedicine. She was the first woman to receive a Doctorate of Science from an Indian university in 1944. Her most notable work includes research on vinca alkaloids, anti-epileptic drugs, and anti-malarial compounds derived from Indian medicinal plants. Chatterjee graduated with honors in chemistry from Scottish Church College in 1936 and earned her master's and D.Sc. from the University of Calcutta. She conducted post-doctoral research on alkaloids in the U.S. with László Zechmeister. Despite facing financial challenges and personal losses in 1967, she continued her research and developed the widely used anti-epileptic drug 'Ayush-56' from Marsilea minuta. She also led work on anti-cancer drugs and founded the chemistry department at Lady Brabourne College. Asima Chatterjee's dedication and resilience made her a trailblazer for women in Indian science.

***Dr Bhupati Chakrabarti*** *is a retired faculty from the Department of Physics, City College, Kolkata and was the General Secretary of IAPT from 2013 to 2018. He can be reached through chakrabhu@gmail.com*

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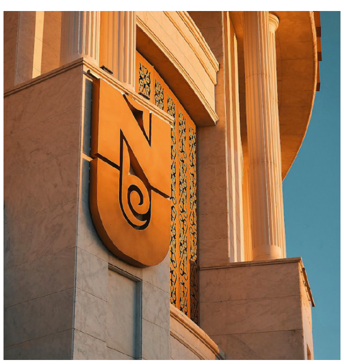

*To walk through the corridors of NU is to witness a vision unfolding —a university that is already Central Asia's finest, now ascending into the ranks of the world's best, with a dream to become the global meeting place of 150,000 young minds.*

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In the very heart of Eurasia, where the winds of history once carried caravans along the Silk Road, stands a modern beacon of learning and discovery—Nazarbayev University (NU). Rising from Astana, Kazakhstan's capital, NU is more than a campus; it is a movement, a declaration that world-class education and research can flourish in Central Asia and shine brightly on the global stage.

From its foundation, NU was never designed to be ordinary. Admission here is purely merit-based, ensuring that the brightest minds from Kazakhstan and beyond find their place within its walls. From the first day of their freshman year, students are immersed in an ecosystem where teaching and research are seamlessly intertwined. Professors do not simply lecture; they ignite curiosity, guide inquiry, and invite students into the living, breathing world of discovery.

## Research at the Core of NU

NU's defining strength is its unwavering commitment to research excellence. Laboratories here are not mere facilities; they are sanctuaries of invention where students and faculty together explore the unknown—whether in artificial intelligence, biotechnology, energy, environmental science, or policy studies. Research is not postponed to graduate school; it begins from the very first year. This spirit has placed NU's scholars and students in leading international journals, collaborative global networks, and at the forefront of solutions to humanity's most urgent challenges.

## A Faculty Beyond Compare

Behind every breakthrough lies NU's extraordinary faculty. With professors hailing from 57 nations, each holding a Western-type PhD or its highest global equivalent, NU has built an intellectual community unrivaled in the region. Its 520 full-time faculty, 27 postdoctoral researchers, and 48 teaching assistants embody both scholarly rigor and global diversity. Many are decorated with awards, fellowships, and memberships in prestigious academies, bringing to NU a vibrancy that blends the traditions of Cambridge, Penn, Singapore, Duke, Wisconsin, and beyond into the unique tapestry of Kazakhstan's academic landscape.

## Number One in Central Asia – Now a Rising Global Leader

The world has taken note. In the Times Higher Education (THE) World University Rankings 2025, NU proudly holds the title of #1 university in Central Asia, a recognition of its excellence and impact. More remarkably, NU has surged ahead to secure a coveted position within the world's top 200 universities—a feat few institutions of such youth have ever achieved.

This ascent affirms what NU has believed from the beginning: that with vision, meritocracy, and relentless pursuit of knowledge, Central Asia can create a university that rivals the world's greatest.

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Yet NU's story is only just beginning. Looking to the horizon, the university has embraced an audacious vision—to welcome more than 150,000 international students over the next three years. This goal is not simply about numbers; it is about transforming Kazakhstan into a global hub of education, where students from every continent gather, learn, and collaborate. In doing so, NU seeks to build not only classrooms without borders but also bridges between cultures, economies, and ideas.

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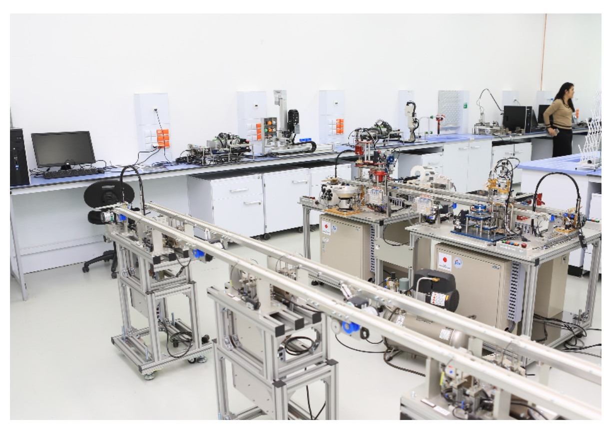

## The Road Ahead

Guided by its Strategy 2018–2030, NU continues to set benchmarks not just for Kazakhstan, but for the world. By 2025, it aims to grow its student body to 8,000 on campus, while simultaneously expanding its global reach through partnerships, online initiatives, and its bold push for internationalization.

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