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Per-Olov Löwdin

Father of Quantum Chemistry

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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**

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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. ◆

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