Professor Axel D. Becke (1953-2025)

Professor Axel Becke, Harry Sherriff Professor of Chemical Research (Emeritus), one of Dalhousie's most impactful researchers, and one of Canada's top scientists, passed away on October 23, 2025, in Halifax.

Axel Dieter Becke was born in Nellingen, Germany in 1953, and came to Canada with his parents at age 3, landing in Halifax. He was the first of four brothers, and from the early days of his life, it would become apparent that he would be first in whatever he decided mattered to him.

His parents, Helmut and Hannelore, created a supportive and nurturing life and learning environment for the family. As Axel wrote for a celebration of life for his father just a few weeks before Axel's own death, "my parents instilled in me a love and curiosity for science as far back as I can remember. Christmas gifts were educational, not just for fun. Meccano sets and Lego sets. Chemistry, electronics and physics sets. Dad found a chemistry textbook at work once, gave it to me – I devoured it from cover to cover." He was a tinkerer in his early life, spending much time by himself building things and playing with machines and gadgets. But as his studies in physics progressed, he became more interested in where formulas came from, and in the theories behind them.

While he made quantum leaps, and quantum chemistry became his life's work, Axel had other early interests in life in which he excelled. In 1970 he leapt almost 23 feet to set a Canadian age class record in the long jump. He won the Canadian Accordion Competition. He had the top marks out of high school and went on to win the gold medal in Engineering Physics at Queen's University. He was always the best at what he did, in all matters, and later, in the study of the motion of electrons in all matter, as a leader in density-functional theory.

Axel spent his entire career in Canada: BSc in Engineering Physics (1975) from Queen's University; MSc (1977) and PhD (1981) in Physics from McMaster University (with Professor D.W.L. Sprung, supported by an NSERC 1967 Science Scholarship); Killam Postdoctoral Fellow (1981-83) and Eastburn Postdoctoral Fellow (1983-84) at Dalhousie University with Professor Russell J. Boyd; first independent academic career at Queen's University (Assistant Professor 1984-89; Associate Professor 1989-94; Professor 1994-2006); and, from 2006 until his retirement in 2015 (when he

was appointed Emeritus), he was Professor and Killam Chair in Computational Science, and Harry Shirreff Professor of Chemical Research at Dalhousie University.

Axel received many awards and honours, including an NSERC University Research Fellowship (1984-1994), 1991 Medal of the International Academy of Quantum Molecular Science, 1994 Noranda Lecture Award of the Canadian Society for Chemistry, 1999 Queen's University Prize for Excellence in Research, 2000 Schrödinger Medal of the World Association of Theoretical and Computational Chemists, Killam Research Fellowship from the Canada Council for the Arts (2005-2007), Killam Chair in Computational Science at Dalhousie University (2006-2016), 2009 John C. Polanyi Award of the Canadian Society for Chemistry, Harry Shirreff Professor of Chemical Research (2011-2015), 2014 American Chemical Society Award in Theoretical Chemistry, induction in the Discovery Centre's Nova Scotia Science Hall of Fame in 2015, the Chemical Institute of Canada Medal in 2015, and the Canadian Association of Theoretical Chemists Honorary Lectureship in 2017. He was a Fellow of the Chemical Institute of Canada, Fellow of the World Association of Theoretical and Computational Chemists, Member of the International Academy of Quantum Molecular Science, Fellow of the Royal Society of Canada (elected 2000), and Fellow of the Royal Society of London (elected 2006). Professor Becke was recognized with the very highest scientific honours in Canada: both NSERC's Gerhard Herzberg Canada Gold Medal for Science and Engineering in 2015, and the Canada Council Killam Prize in the Natural Sciences in 2016.

These awards were in recognition of Axel's transformative scholarship in the field of quantum chemistry, with significant impacts in many fields of science. Methods developed by Axel Becke are used worldwide, by all major pharmaceutical companies for the development of drugs, by the petrochemical industry for the design of better catalysts, and by many other industries and academics for the development of new materials. Even NASA scientists employ Becke's computational methods to support their space exploration programs through modelling of materials.

In 2014 the journal *Nature* compiled a list of the 100 most-cited scientific papers of all time. Numbers 8 and 25 were single-author papers by Becke. These two seminal papers continue to be cited and are generally acknowledged to have been instrumental in the awarding of the 1998 Nobel Prize in Chemistry to Walter Kohn and John Pople. Pople and Kohn never missed an opportunity to cite and acknowledge Axel's contributions to the field.

Axel's first conference presentation was in Halifax in June 1981 at the 64th Canadian Chemical Conference. The one-day symposium on theoretical chemistry, organized by Russell Boyd, opened with a keynote lecture by John Pople and concluded with a brilliant lecture by a then-unknown Axel Becke. Many of the participants later asked the organizer, "Who is that guy?". Axel never forgot when and where he met John Pople, who in turn followed Axel's work very closely and supported Axel's successful nomination as Fellow of the Royal Society of London.

Axel was not just an impactful researcher, he was also a talented teacher. His lectures were clear and engaging, even when the subject matter was very difficult. He won the Queen's Chemistry Department Student Council Award for Excellence in Teaching (1987) and the Queen's University

Engineering Society “Golden Apple” Award for Excellence in Teaching (1992). He was happy to teach, as long as it was not early in the morning.

Axel was no doubt brilliant, persistent and determined, but if you met him, you would find him to be thoughtful, pleasant, and unassuming. Kind and gentle.

Axel loved the outdoors. He enjoyed the many parks, ocean vistas and destinations the Halifax area offers. Earlier in his life, he treasured the annual Algonquin Park family camping trip. As a teenager, he went on canoe trips that were certainly not leisurely, mountain hikes that felt like a time trial. It was always hard to keep up with him…

Axel was laid to rest in Oakridge Memorial Gardens, Halifax. At the top of the hill.