NEW MATERIALS DESIGNED BY ARTIFICIAL INTELLIGENCE

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When I compare university textbooks from half a century ago with the latest editions fresh off bookstore shelves, I notice a striking difference in design and illustration. Yet, the core scientific concepts remain largely unchanged. Mechanics and magnetism in old physics books, thermodynamics and kinetics in chemistry, or differential equations in calculus—these fundamentals have withstood the test of time.

In contrast, the tools on my current office desk are dramatically different from those on my first desk over fifty years ago. This raises an important question: if fundamental science hasn't changed, what has driven the transformation in our tools and technologies?

The answer lies in materials and processing. New materials have enabled the creation of novel tools, while new processing have allowed us to engineering these materials in ways that were once unimaginable—unlocking functionalities that were merely dreams half a century ago.

This seminar at first offers a brief overview of the development of several advanced materials that have driven these changes. Materials such as organic and inorganic compound semiconductors, high-temperature superconductors approaching room temperature, or photovoltaic materials for efficient solar energy conversion—though known for a long time—have only recently entered commercial applications. Most of these breakthroughs stemmed from intuition, persistent experimentation, and trial-and-error methods.

After decades of research, vast libraries of compounds, structures, and phase diagrams now fill databases. However, it is clear that these databases cover only a small portion of the possible materials universe. For example, between two elements A and B, about 5000 binary combinations are possible, and nearly all binary thermodynamically stable phase diagrams have been published. But theoretically, over 160,000 ternary compounds of the form ABC could exist—most of which are still unknown, with their properties unexplored.

In recent years, the introduction of artificial intelligence (AI) into materials science has revolutionized the way we design new compounds and structures. Programs such as DeepMind's AlphaFold, which hosts approximately 200 million predicted protein structures, and Microsoft's MatterGen, which can generate structures for a vast array of potential compounds, exemplify this shift. This leads to a legitimate question: what remains to be done in materials science?

What is already evident is that AI-based tools are rapidly becoming indispensable in the design of new materials and should be considered standard equipment in every modern materials science laboratory. At the same time, it is important to recognize that while AI excels at prediction, validating these results still requires rigorous experimentation—and surprises are still possible. One such example is the recent (2025) discovery of superconductivity near 40 K in $SmNiO_2$, which was not predicted by AI.

CHRISTIAN KLOC was a tenured professor in the School of Materials Science and Engineering at the Nanyang Technological University (NTU) in Singapore. He joined NTU in 2007 and ran a crystal growth laboratory with undergraduate and graduate students as well as postdocs. His research focused on structure–property relations and charge transfer in multicomponent organic and inorganic compounds.

In 1974, he received his chemical engineering degree from the Technical University in Gliwice, Poland. He then joined the Solid State Physics Institute of the Polish Academy of Sciences in Zabrze and earned his Ph.D. in physics from the Institute of Physics of the Polish Academy of Sciences in Warsaw.

In 1982/83, he was a postdoctoral fellow at the University of Braunschweig, Germany, working under Prof. Dr. Rolf Lacmann on the electrocrystallization of metals. From 1986 to 1998, he worked with Prof. Ernst Bucher at the University of Konstanz, Germany, focusing on the crystal growth of semiconductors and intermetallic compounds.

Starting in 1991 as an exchange scholar, and from 1998 until 2007 as a permanent researcher, he conducted research in the Physical Research Department at Bell Labs in Murray Hill, New Jersey, where he explored new materials ranging from superconductors and magnetic/insulating materials to organic and inorganic compound semiconductors.

He has special expertise in growing novel single crystals that are not commercially available. Prof. Kloc has published over 200 papers and, as of 2025, has 26,000 citations and an h-index of 73, according to Google Scholar. Since his retirement, he has been living in Heidelberg, and his recent interests include the application of artificial intelligence to materials science.