

Wolfgang Moritz FREE

25 August 2025

(24 September 1943 – 29 October 2024)

The German physicist was a pioneer in quantitative surface structure determination, using mainly low-energy electron diffraction and surface x-ray diffraction.

[Michel A. Van Hove and Ian Robinson](#)

DOI: <https://doi.org/10.1063/pt.jwww.ggan>

Wolfgang Moritz, former professor of physics at the Ludwig Maximilian University of Munich (LMU), died on 29 October 2024 at the age of 81. Wolfgang had a distinguished career in surface science, developing advanced methods of surface structure analysis by means of low-energy electron diffraction (LEED) and surface x-ray diffraction (SXRD).

Wolfgang was born near Berlin in 1943. After undergraduate studies in physics at the Technical University of Berlin, he completed his doctoral thesis at the LMU (1976). He then became research associate at the Institute of Crystallography and Mineralogy of the LMU, where he obtained his habilitation (1984).

Wolfgang was a visiting scientist at the University of Wisconsin–Madison (1984–85) and in 1986 returned to LMU as professor in the department of physics and later in the department of Earth and environmental sciences. After retiring in 2008, he remained highly active in research. Despite his cancer, Wolfgang lived to witness the success of his book *Surface Structure Determination by LEED and X-rays* (published in 2022 with Michel Van Hove).

Wolfgang was among the few who went beyond determining atomic coordinates and bond lengths. He was also very interested in



(Photo courtesy of the authors.)

quantitative studies of nonstructural aspects of surfaces, such as thermal vibrations, and various kinds of disorder and defects.

For his PhD thesis, Wolfgang studied LEED from disordered surfaces. With collaborators Heinz Jagodzinski and Dieter Wolf, he published the first accurate treatment of multiple scattering in diffuse LEED from disordered surfaces. Some of those ideas were later used by others in SXRD, photoelectron diffraction, and surface EXAFS.

From 1991, Wolfgang became heavily involved in x-ray diffraction from surfaces, collaborating with Robert Feidenhans'l, Robert Johnson, Xavier Torrelles, Ian Robinson, Holger Meyerheim, and others. They greatly refined the experimental and theoretical methods of surface x-ray diffraction. In particular, Wolfgang built an in-house surface x-ray diffraction instrument for ultrahigh vacuum that could be transported to synchrotron radiation facilities.

In the 1990s, Wolfgang became interested in the anisotropy and anharmonicity of thermal vibrations of surface atoms and molecules. For example, with Herbert Over and Gerhard Ertl, he studied CO on Ru(0001) by LEED, finding CO to be tilted on the average by 12° at 150 K due to bending vibrations. Using SXRD, together with Meyerheim and Robinson, he found anharmonic thermal vibrations of Cs adsorbed on Cu(001).

Wolfgang analyzed incommensurate layers, such as graphene on a metal substrate. Those layers in particular can buckle due to varying placements of their atoms over the substrate atoms.

With Meyerheim, he studied systematically how antiphase domain structures result from strong interactions between overlayer and substrate; that work has widespread implications in magnetic recording technology, for example.

Wolfgang worked on direct methods, such as the “structure completion problem.” With Dilano Saldin and Robinson, he developed a method called Phase and Amplitude Recovery and Diffraction Image Generation Method (PARADIGM). It is a variation of Fienup’s iterative input–output feedback method for the phasing of surface x-ray diffraction amplitudes that relies on successive transformations between real and reciprocal space.

Wolfgang and Van Hove were friendly competitors in the structure determination of C_{60} on metal surfaces, by LEED. Wolfgang’s team won, including the efforts of Renee Diehl, Katariina Pussi, and Ronan McGrath. They found that C_{60} on Ag(111) forms a remarkable one-atom hole in the metal surface. (The competing study found seven-atom holes for C_{60} on Cu(111). Both results were confirmed later.)

Finally, Wolfgang worked on a more theoretical aspect of LEED with John Rundgren and Bo Sernelius: The muffin-tin potentials used to describe electron scattering are generally assumed to not overlap, causing artificial steps in the potential and artificial scattering. By

using overlapping spheres, they produced an entirely step-free scattering potential and, consequently, the agreement between LEED theory and experiment was significantly improved.

Wolfgang was both an accomplished theorist and an accomplished experimentalist, a rarity in the field of surface science. He was an avid trekker, skier, cook, and arts devotee. Wolfgang was humble, self-effacing, generous, and a great friend with mischievous humor. He was very knowledgeable and highly reliable, very systematic and meticulous, as well as opinionated. He greatly enjoyed collaborating with students and other colleagues. Wolfgang and his wife also generously assisted refugee children.

Wolfgang's wisdom, insight, generosity, and friendship will be sorely missed.

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