Walter Kohn

(1923–2016)

Condensed-matter physicist who revolutionized quantum chemistry.

Walter Kohn's profound questioning of what the arrangement of electrons can tell us about a material's character led to density functional theory. The theory, which predicts electron energies, became a basic tool in efforts to compute the properties of materials and the outcomes of chemical reactions. Some say that it revolutionized quantum chemistry, the application of quantum mechanics to the study of molecules.

Kohn, who died on 19 April, was born in Vienna in 1923. In 1939, not long after the annexation of Austria by Nazi Germany, Kohn's parents sent him to England on a convoy of the *Kindertransport*, an operation to rescue Jewish children from Europe before the outbreak of the war. His mother and father were later killed at Auschwitz.

In 1940, as a holder of a German passport, Kohn was shipped to the first of what would be a series of internment camps in Canada. Once free to leave, he began studies at the University of Toronto, where he earned a bachelor's degree in mathematics and physics and master's degree in applied mathematics. In 1948, he completed a PhD in nuclear physics at Harvard University in Cambridge, Massachusetts; his supervisor was the Nobel-prizewinning theoretical physicist Julian Schwinger.

In 1950, after a short stint of postdoctoral work, Kohn took a professorship at the Carnegie Institute of Technology in Pittsburgh, Pennsylvania (now Carnegie Mellon University). A decade later, he joined the physics department at the University of California, San Diego, where he worked for nearly 20 years before becoming the founding director of the Institute for Theoretical Physics at the University of California, Santa Barbara (now the Kavli Institute).

A condensed-matter system, from a single atom to a living organism, is composed of nuclei and electrons. The electrons roam in an energy landscape provided by the nuclei, and each electron is influenced by the others. The electrical charges of any pair of electrons in the same energy landscape interact, and no electron can exist in the same state as another in the same energy landscape (the Pauli exclusion principle).

In the 1950s and 1960s, physicists were using two different approaches to compute the energy states of electrons in a material. In both approaches, the energy landscape was thought to be key to the prediction of

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the properties of a system, including the distribution of electron density. The density functional theory swapped the cause and effect roles between the energy landscape and the electron-density distribution. This paved a way to compute the properties of functional importance to technologies and to life, such as electronics and photosynthesis.

Around 1960, Kohn started to examine the change that occurs to the spatial distribution of the electron density when an impurity is added to a metal. For a positively charged impurity, the electrons pile up around it as expected. They also exhibit a wave-like distribution (Friedel oscillations), which reflects a quantum property of the electrons. This quantum feature led Kohn to examine the possibility that the electron density contained the key to other properties. In 1964, while on sabbatical in Paris, he established with Pierre Hohenberg, a postdoc at the École Normale Supérieure, the Hohenberg–Kohn density theorem. This stated that the electron-density distribution (not the energy landscape) determines the properties of a many-electron system.

Returning to San Diego, Kohn prompted a postdoc, David Mermin, to generalize the theorem so that it could be applied to all temperatures. In 1965, he established with another postdoc (me) a way to use density functional theory to compute the properties of materials.

Kohn's PhD student at San Diego, Philip Tong, was the first to apply density functional theory to infer the electron energies of atoms of noble gases and of the sodium lattice. With his postdoc, Norton Lang, Kohn applied the theory to calculate properties of metal surfaces in the early 1970s. Kohn and Lang won the Davisson–Germer prize in 1977 for their contribution to surface physics. For his work on density functional theory, Kohn shared the 1998 Nobel Prize in Chemistry.

For several years after the Hohenberg–Kohn theorem was published, theoretical chemists raised objections — almost unanimously — to the central role of the electron-density distribution. They could prove that a more general property known as the density matrix was the fount of all electronic properties. They thought that the electron-density distribution, which was only a component of this matrix, could not offer the same predictive power. In the end, people were persuaded by the simplicity of the proof of the theorem, and by the efforts of numerous researchers who showed its usefulness.

Walter was meticulous in his research — but in sports he was adventurous. In 1996, he wrecked his shoulder skiing the day before a widely anticipated talk on density functional theory at an annual meeting of the American Physical Society, and asked me to speak in his stead. He said that he had used a mogul to launch a jump, recalling the ski jumps he had made as a child in Austria. On another occasion, he took his eldest daughter, Marilyn, and me sailing beyond the surf at La Jolla Shores beach in California on a windy day. The boat capsized, and as we pushed it back towards the beach the surf ripped it from our hands.

Walter cared deeply about social issues. At San Diego, he promoted the Judaic studies programme. He was also a vocal critic of the University of California's association with the national weapons laboratories in Los Alamos, New Mexico, and in Livermore, California. And he was proud of producing a documentary film promoting solar energy.

Walter was an admired mentor and colleague, and will be missed by the many who came within his orbit. ■

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