Max Planck Institute for Solid State Research

Ove Jepsen died suddenly on January 4th at age 73. He was an internationally recognized pioneer of electronic-structure calculations. From 1979 until beyond his retirement in 2011 he worked at the Max-Planck Institute for Solid-State Research in Stuttgart where he contributed significantly to the friendly, international atmosphere, had many collaborations across departments, and was highly respected.

Ove obtained a PhD from the Technical University of Denmark in 1972. His thesis on the Fermi surface of Yb included The Tetrahedron Method and was published in Solid State Communications. At the 40th anniversary of that journal, this paper had become its second most cited, and together with papers from 1984 and 1994 containing improvements of the method it has now been cited 5000 times. Ove joined the Danish National Laboratory at Risø where in 1973-75 he wrote the first LMTO-ASA band-structure code enabling density-functional (DF) calculations for *s*-, *p*-, *d*-, and *f*-electron materials. With it, he first demonstrated that spin-polarized DF theory accounts for the pressure-volume relations of iron in the closely-packed phases, and later he treated all elemental metals. For transition-metal surfaces, accurate DF calculations became possible thanks to Ove's full-potential LAPW code developed a few years later when he was at NORDITA in Copenhagen. In 1978, Ove was invited to Cornell University where he met Virginia. They married in La Paz, Bolivia, and moved to Stuttgart in 1979.

In the newly formed department for electronic-structure calculations Ove became responsible for developing, maintaining, and using the codes, and for teaching the students and the many post docs who over the years came from in particular Italy, Japan, North- and South America, Eastern Europe, Russia, Ukraine, India, and China. Also privately, he and Virginia cared for the young scientists, and many life-long friendships were formed.

The Stuttgart TB-LMTO-ASA code was probably the first DFT code made freely available. Ove was the one who showed that the transformation to tight-binding (TB) works, and the corresponding PRL from 1984 became his second-most cited paper (2500 times). The TB feature not only made DF calculations possible for condensed matter without 3D periodicity, but also made the band-structures intelligible. This became essential as the discovery of high-temperature superconductivity in cuprates (HTSC) necessitated an improved treatment of electronic correlations. Ove calculated the parameters of the Anderson impurity Hamiltonian, a prerequisite for the later development of the LDA+U method in the department and, eventually, for the first *ab initio* applications of dynamical mean field theory (DMFT). Also the development of electronic indicators, specifically Canonical Bands, Fat Bands, ELFs, and COHPs were facilitated by Ove. Properties treated by Ove and collaborators included Fermi surfaces, chemical binding, magnetism, optical properties, and electron-phonon mediated superconductivity. He calculated and analyzed the electronic and phononic structure of numerous materials of current interest, most notably HTSCs, A_3C_{60}, and MgB_2. To date, Ove's papers have been cited ˜25 000 times and his h-index is ˜60 (Google Scholar).

He co-organized the 1st and 2nd Psik conferences which took place in Schäbisch Gmünd 1996 and 2000. In 2008, he was selected as Outstanding Referee for the Journals of the APS.

Ove loved and was proud of his family: Virginia, Marianne and Charlotte. He was also proud of being a Dane. On Fanø, a sandy island outside the Danish west coast, he owned a summer house, where he and his family spent the summer every year. Friends were very welcome there, too. Ove also enjoyed reading a good book, travelling, playing tennis, and was interested in art and music.

Many will miss him.