

In Memory of Jaap G. Snijders (1951-2003)

Published online 28 April 2006 in Wiley InterScience (www.interscience.wiley.com).
 DOI 10.1002/qua.21037

Jaap Snijders began his academic career in 1968 studying chemistry at the University of Amsterdam. He graduated cum laude in 1973. He then moved to the University of Sheffield, UK, for 2 years to do research with Professor Roy McWeeny.

After returning to Amsterdam, he started doctoral research under the guidance of Professor Piet Ros, at the Free University. He defended his thesis, entitled "Relativity and Pseudopotentials in the Hartree-Fock-Slater Method," in 1979. He then stayed on at the university, first as Assistant Professor (*docent*) and later from 1986 as Associate Professor (*hoofddocent*).

In 1992 he received a special nomination as professor to teach quantum chemistry of spectroscopic phenomena, which he accepted with a lecture (*oratie*) entitled "Light on Matter" ("*Licht op de materie*") in 1993. During his 22 years at the Theoretical Chemistry Department of the Free University, he collaborated closely with Professor Evert-Jan Baerends, with whom he worked on density functional theory (DFT).

In 1997 he was appointed Full Professor of Theoretical Chemistry at the University of Groningen as successor of Professor Wim Nieuwpoort. The chair he now headed is part of the Material Science Centre (MSC). He quickly built a group, specialized in the development, implementation, and application of time-dependent density functional theory (TDDFT). He initiated collaborations with MSC colleagues and extended his group with promising young researchers. His group received support from the Dutch organization for scientific research, NWO (Nederlandse Organisatie voor Wetenschappelijk Onderzoek) in the form of a *springplank* fellow and a *Vidi* grant. He



JAAP G. SNIJDERS

supervised seven PhD students during his life; for four of them he was entitled to act as promotor.

Jaap Snijders is coauthor of the widely used Amsterdam Density Functional program, an offspring of the Hartree-Fock-Slater program developed at the Free University. He contributed, for instance, to the parallel implementation of the code. In his recent research, the following main subjects may be distinguished.

His endeavors to incorporate relativistic effects in standard quantum chemical methods, which al-

ready started during his PhD research, resulted in the rediscovery of an approximate two-component relativistic operator, now known as the ZORA approach. This method was incorporated in both a DFT program (ADF) and a wave function-based program (GAMESS-UK).

He had a great interest in scattering theory, both in teaching, he gave lectures at Dutch postgraduate summer schools, and in his studies of the influence of molecular orientation in NO–Ar collisions. The orientation of small molecules, solvated in liquid crystals, as detected by nuclear magnetic resonance (NMR) was another of his interests.

In Groningen, he became interested in the two-dimensional Raman response of atoms and molecules in liquids. The work resulted in the proposal of a special configuration of laser polarizations, a configuration now known in literature as “Dutch cross.” He also joined in the existing research in Groningen on the effects of the environment on biomolecules, using QM/MM techniques.

The last focus of his research was on response properties, especially on methods to calculate them, as it was already formulated in his *oratie* in Amsterdam. He started with employing coupled cluster techniques, but concentrated more recently on TD-DFT. Response functions calculated included dynamic dipole and quadrupole polarizabilities of molecules and dielectric properties of solids.

Jaap’s research was widely respected and appreciated both nationally and internationally. Teaching was very dear to him. He was greatly concerned about the proposed changes in the chemistry curriculum, as he feared that the quality would suffer.

Jaap considered theoretical chemistry in particular as one of the fundamental building blocks of chemistry education, which could not be omitted without destroying the whole building. He used to teach using only a blackboard, which was much appreciated by the students.

At the Free University, Jaap was Secretary and later Chairman of Theoretical Chemistry and member of various committees within and outside the faculty, for example, at the Amsterdam Computer Centre SARA. In Groningen he was a member, and later chairman of the board of the Materials Science Centre. He was secretary of the national NWO study group Spectroscopy and Theory.

Jaap’s presence never went unnoticed. He had strong opinions and liked a good debate, preferably while enjoying good food and drinks. He was a quick and deep thinker and had a thorough knowledge of theoretical and physical chemistry and the mathematics involved. He was well read and had an excellent memory. He was a valued speaker with a nice sense of humor. The many who knew him as colleague, teacher, or supervisor will remember him as a remarkable man en a passionate scientist.

Jaap G. Snijders, Professor of Theoretical Chemistry at the University of Groningen, died August 13, 2003 after a short illness at only 52 years of age in a hospital in Stadskanaal near his beloved home in Gasselte, Drente, The Netherlands. He will be missed.

RIA BROER

JOOP VAN LENTHE

Gröningen, Utrecht, The Netherlands