

Editorial

to the Special Issue of the Journal of Mathematical Chemistry
"In Memoriam János Pipek"



Born in 1954, died in 2021, János Pipek was a widely known quantum chemist, his main affiliation being at the Technical University of Budapest (BME) in an institute founded originally by Pál Gombás. He received his masters (1977) and doctoral (1981) degrees from the Eötvös Loránd University (ELTE), Budapest, Hungary.

As a young scientist, he was working with Professor Ede Kapuy at BME, who supervised János' studies at the beginning. Their relation developed into a long-standing and fruitful cooperation. János was also working with Professor János Ladik in Erlangen, Germany (1982-83), and with Professor Paul Mezey in Saskatchewan, Canada (1987-88), but always returned to BME where he kept permanent position.

The scientific interest of János Pipek can be divided into two distinct parts. The first, more accentuated portion could be characterized as "Localized Molecular Orbitals: Construction and Use". He started to study the properties of localized orbitals, and to apply them in a version of many-body perturbation theory that is nowadays termed as "Davidson-Kapuy partitioning". Some of these results got summarized in the important review: *J.Pipek and F. Bogár, Topics in Current Chemistry, Vol 203, Ed. P.R. Surján, p. 43*. Some of his works addressed the technology of constructing localized orbitals. In the paper with Mezey, a new localization functional was proposed (*Pipek-Mezey localization, 1989*). This paper has received more than 1400 independent citations to date.

János became interested in the potential applications of wavelet analysis in quantum chemistry and published several papers in this field, too.

János Pipek was active in scientific publications both with his students as well as in cooperation with colleagues, but, what appears especially important nowadays, he has several single-authored papers in leading international Journals.

János Pipek lived for Science and hated bureaucracy. He was by no means a careerist. However, when recognizing that it was his time to grab the steering wheel, he never hesitated. He served at the Faculty of Science of BME as a vice dean (1998–2011) and for two periods as the dean (2011–2018).

János had a characteristic, cheerful attitude to life that made it a pleasure to meet him at any time. We won't forget his gentle but sparkling and optimistic personality.

Ágnes Szabados
Péter Suján
guest editors