Theoretical Chemistry Accounts (2018) 137:175
https://doi.org/10.1007/s00214-018-2364-3

EDITORIAL

Editorial: in memoriam János G. Ángyán (1956–2017)

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Received: 6 September 2018 / Accepted: 26 September 2018 / Published online: 15 November 2018

Abstract
Introduction to the honorary volume dedicated to the memory of János G. Ángyán, died too early, on January 22, 2017, at the age of 60. We recall some stations of his life and essential elements of his research.

Keywords Obituary · Editorial

János Ángyán, born in 1956 in Pécs, Hungary, spent his life and career between his hometown Budapest, his permanent office in Nancy, and in close collaboration with colleagues in Paris. It is therefore natural that three editors from these three places cover this honorary volume.

Already, his first (co-)signed publications show his broad vision of theoretical chemistry: As of 1983, we find applied work on antibiotics [1], a mathematical study on perturbation theory for time-independent Schrödinger equations [2], contributions to spectroscopy for optical rotatory strength calculations [3], and the main conductor of his further research, electrostatic potentials in molecular assemblies [4]. Even before having accomplished his thesis, János made contacts to the Paris' research groups, leading to postdoctoral stays in Toronto (Canada) and Paris (France), publishing regularly with colleagues from Hungary [5] and France [6] while being officially a research associate in Budapest, Hungary.

In 1990–1991, he spent 2 years as a Humboldt fellow in the universities of Stuttgart (organic chemistry) and Bonn (theoretical chemistry) in Germany, before entering in 1991 the Centre National de la Recherche Scientifique (CNRS) in the laboratory of theoretical chemistry in Nancy, where he became a research director in 2000, followed by, in 2001–2002, a 1-year stay at the Institut für Materialphysik of the University of Vienna, Austria, as a guest professor. In 2004, he moved to the Laboratory of Crystallography, Magnetic Resonance and Modelisation (CRM2) in the University Nancy I (now part of the University of Lorraine) in France. Recently, in 2016, he was elected external member of the Hungarian Academy of Sciences.

During this time, he published around 130 scientific papers with a large number of co-authors in different fields, supervised around a dozen of doctoral theses, and participated in the management of science as member of editorial boards (in particular of the present journal from 2000 to 2008), evaluation commissions, and organizer of various scientific meetings. Together with Bernard Silvi, he managed for instance in 2001 to gather around 70 scientists in Colle-sur-Loup in the south of France to discuss possible strategies to interpret chemical bonds with mathematical tools and a chemical language [7], known today as "conceptual DFT," and various indicators like Bader's theory of atoms in molecules or electron localization functionals.

Along his scientific career, Janos has been interested by a wide panel of topics—among them are the static and inductive electrostatic interactions in condensed media which are the common theme of many of his published

Published as part of the special collection of articles in memoriam of János Ángyán.

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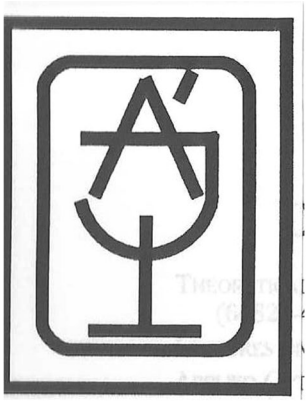
works. He was particularly interested in the construction of models involving distributed multipole moments and distributed multipole polarizabilities, which lead for example to the optimally partitioned electric properties (OPEP) code [8]. The fast evaluation of accurate molecular electrostatic potentials is a challenging problem for the modeling of chemical systems in condensed media, and many charge fitting methods have been developed for this purpose. In order to go beyond this technology, Janos, among others, has proposed models in which electric multipoles are distributed over fragments [9–11]. He had examined methodological aspects of this problem analyzing the accuracy of the different distributed multipole and point charge models [12–17]. Even more important is his contribution to the calculation of induction and dispersion energies from distributed polarizabilities initiated in 1994 within the QTAIM partition scheme [18], resulting in the TPEP (topologically partitioned electric properties) program [19]. He further thoroughly investigated the properties of distributed polarizability techniques [20–27]. In the same way, he has addressed the calculation of dispersion energy from distributed dynamic polarizabilities. For all of these distributed quantities, his priority was to devise efficient methods without searching for physicochemical interpretation of individual numbers.

A vast field of applications of these functional and series expansions is the treatment of dispersion interactions in a density functional framework. In this context, in the quest to improve systematically density functional theory, he collaborated closely with A. Savin on range-separated DFT, publishing fundamental studies on perturbation theory [28, 29] and the random-phase approximation (RPA) [30], leading to various implementations for the molecular case (in the program package Molpro). Following his stay in Vienna, he broadened his expertise to include solid state physics: For instance, he contributed to the implementation [31] of the RSHX functionals in the VASP code and to a study [32] of the cohesive properties of graphite using RPA. Also, he initiated the implementation [33] of Grimme's D2 correction in the same code, a work which was the beginning of a series of papers [33–36] on the implementation of different schemes to correct for the missing dispersion forces of local and semi-local density functionals in solids. Those features are now widely used by the VASP community. Related to these topics, one of the last meetings he organized was a CECAM workshop in Nancy in June 2016, entitled "Density- and response density-based models for Intermolecular Interactions in Molecular Assemblies and in Solids."

Besides his scientific activities, we remember a lively person, open to discuss and to animate, with a strong interdisciplinary, international, and cultural background, summarized in one of his *ex libris* designed by himself.



In the present volume, we could collect in 33 articles many of the different facets of János' work, ongoing collaborations with colleagues all over the world, having come too soon to an end, and ideas which may be further developed. He left us, but souvenirs and achievements will remain.

We thank all contributors and referees for their work, and Mrs. Ananthanarayanan of Springer for her patience in handling the manuscripts.

Paris–Nancy–Budapest, August 2018.

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