

FOREWORD

## Foreword for special issue of Molecular Physics in honour of Andreas Savin

Andreas Savin was born on 20 April 1950 in Bucharest (Romania), where he grew up during the communist era in a German-speaking family. From an early age, he was exposed to several languages (German, Romanian and French).

Andreas began his research in theoretical chemistry at the Polytechnic Institute in Bucharest in the late 1970s. In 1977, he published his first paper, on the application of semiempirical methods to the stability of aromatic hydrocarbons, followed by several papers on the use of localised molecular orbitals.

In the early 1980s, escaping from the Ceausescu dictatorship, Andreas moved to the Institut für Theoretische Chemie at the University of Stuttgart in Germany. There, he started to work on density-functional theory (DFT) and pseudopotentials, as a Ph.D. student under the supervision of Heinz Werner Preuss and Hermann Stoll. He was among the pioneers developing and testing correlation density functionals at a time when DFT was unpopular in quantum chemistry. He defended his thesis 'Die explizite Behandlung von Korrelationseffekten in Dichtefunktional- und Pseudopotentialmethoden' (The explicit treatment of correlation effects in density-functional and pseudopotential methods) in 1983.

After gaining his Ph.D., Andreas continued to work in Stuttgart, mostly on DFT and pseudopotentials. In particular, he began to develop the idea of combining the configuration-interaction (CI) method with DFT, which became the central theme of his Habilitation 'Eine Kopplung der Konfigurationswechselwirkungsmethode mit dem Dichtefunktionalverfahren' (A coupling of the configuration-interaction method with the density-functional method) that he obtained in 1988.

In the early 1990s, Andreas started new research directions. He published in 1991 (with Axel Becke, Jürgen Flad, Reinhard Nesper, Heinz Werner Preuss and Hans Georg von Schnering) his first paper of a long series on chemical bond analyses using the electron localisation function (ELF), which had been introduced one year earlier. In 1992, he published with Heinz-Jürgen Flad and Heinz Werner Preuss his first paper on improvements of the quantum Monte Carlo method for quantum chemistry.

In 1993, Andreas moved to Paris with a CNRS (French National Research Center) research position at the Laboratoire de Dynamique des Interactions Moléculaires, which later became the Laboratoire de Chimie Théorique,

of the Université Pierre et Marie Curie. There, he initiated with Bernard Silvi the topological analysis of ELF. He also continued his work on DFT, and, in 1995, he published a series of papers on the interpretation of broken-symmetry spin DFT in terms of the on-top pair density, together with John Perdew, Kieron Burke, Axel Becke and Hermann Stoll. In the same year, he published with Heinz-Jürgen Flad the first paper introducing the rigorous formalism of range-separated DFT, combining wave-function theory and DFT by a range separation of the electron–electron interaction – an idea first put forward in a book chapter published with Hermann Stoll in 1985. This first variant of range-separated DFT used the Yukawa interaction. The now standard error-function interaction in range-separated DFT was introduced by Andreas in 1996.

In the late 1990s and early 2000s, while still developing methods combining wave-function and DFT approaches, Andreas began to explore properties of exact DFT. With François Colonna and other collaborators, he was among the first to calculate accurate Kohn–Sham potentials along the adiabatic connection. At the same time, he continued to work on chemical interpretation methods. In 2002, he published his first paper on calculating explicit probability distributions to analyse electron localisation. With several collaborators, he later developed this work into what is known today as the maximum probability domain method.

Andreas' most recent work includes further developments of range-separated DFT – in particular, using extrapolation schemes along the adiabatic connection – and the exploration of the pitfalls of statistical analyses in benchmarking methods.

In this special issue of Molecular Physics, Andreas' friends and colleagues contribute to the celebration of his 65th birthday by publishing their most recent work in the area of electronic-structure theory. Andreas' infectious enthusiasm and willingness to openly share scientific thoughts and ideas continue to inspire further progress in the field. We wish him all the best for the future and look forward to many more years of his friendship and creative science.

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