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Special Issue of Molecular Physics in Honour of Professor Johann Fischer

Rolf Lustig, Carlos Vega & Jadran Vrabec (Special Issue Editors)

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FOREWORD



Special Issue of Molecular Physics in Honour of Professor Johann Fischer

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It is a great pleasure to celebrate the 75th birthday of Professor Dr. phil. Johann Fischer with this body of work in a Special Issue of *Molecular Physics*. Numerous warm-hearted responses that we have received during the organisation of this issue are testament to the great respect that he has earned as a person. The contributors to this issue reflect the broad influence Johann Fischer's work has had (and is continuing to have) on the scientific community, representing a wide field ranging from fundamental Statistical Thermodynamics to applications in Engineering.

Born on 31 August 1942 in Amsterdam, at age five Johann Fischer's family relocated to Wien (Vienna), where he spent most of his youth. After graduating from secondary school in 1960, he started studying physics and mathematics at Universität Wien to become a teacher. He was awarded a Fellowship of the French Government at that time. In 1966, he became Scientific Coworker at the Institut für Physikalische Chemie, Universität Wien. His dissertation on cell theory for liquids, which he defended in 1971, was supervised by Professor Dr. Friedrich Kohler. Shortly after, he became Assistant Professor at the Institut für Theoretische Physik, Ruhr-Universität Bochum. As a consequence of this appointment and his contact with Professor Dr. Gerhard H. Findenegg he began research on molecular modelling of fluids at surfaces. It was unusual for the doctoral advisor to follow the student from Wien to Bochum with the result that Johann Fischer became Akademischer Rat at the Institut für Thermo- und Fluidodynamik, Ruhr-Universität Bochum in 1977. Once more, Professor Kohler became Johann Fischer's mentor; this time for his Habilitation thesis in statistical thermodynamics of fluids in equilibrium at interfaces, which he defended in 1981. Five years later, he was promoted to Professor. In 1994, he accepted a call to become Professor of Mechanical and Energy Engineering at Universität für Bodenkultur Wien. There, he headed the Institut für Verfahrens- und Energietechnik from 2004 until his retirement in 2008. Since then, he has been actively conducting research as Professor Emeritus.

Johann Fischer married Ruth Pollmann in 1969. Their daughter Eva was born 1971 in Wien and their son Christian 1974 in Bochum. Eva currently lives in Melbourne and Christian in Innsbruck.

Johann Fischer and his collaborators have authored 127 peer-reviewed papers in prestigious international journals to date, 25 of which are in *Molecular Physics*. He began publishing in 1967 on the cell theory of liquids. He posited broad fundamentals through his contributions to the book 'The Liquid State' by Friedrich Kohler, which appeared in 1972. The broadness of his outlook to science is reflected by numerous publications in varying fields; such as electrophoresis, group-contribution theory of mixtures and the thermodynamics of hard bodies.

From 1975 throughout his career, Johann Fischer worked on various aspects of adsorption, employing different approaches, including integral equations, density-functional theory and molecular simulation. His work on the use of integral equation theory of fluids in contact with a surface is one of the first of its kind [1]. One particular interest originated in 1979 [2], and spanned over almost two decades: Johann Fischer contributed significantly to the fundamentals of perturbation theory for molecular liquids and their mixtures, including the accurate description of vapour-liquid equilibria (for example, see [3,4]).

The firmly theory oriented Johann Fischer was initially quite sceptical about molecular simulation. However, in the mid-1980s, he became more open toward this emerging new tool, to which he would later contribute significantly both fundamentally and practically. Johann Fischer was the first scientist in Germany who gave graduate students in engineering the opportunity to work in this unfamiliar field, which at that time was viewed by many with scepticism. All three of the Special-Issue Editors were involved in that crucial period of change and benefitted greatly. Johann Fischer applied the statistical approach to the thermodynamic properties of many compounds and their mixtures (e.g. natural gases and refrigerants [5]). He paid special attention to improvements of combining rules in molecular mixtures.

An important methodological achievement was the NpT + test particle method, which was published in 1990 for the molecular simulation of vapour–liquid equilibria by the group of Johann Fischer [6]. His results for the Lennard-Jones system from 1992 are still considered as the ultimate standard for accuracy [7]. The method was subsequently extended to binary and ternary mixtures. In parallel, he worked on vapour–liquid equilibrium simulations of phases in direct physical contact; a topic that he has contributed to in different forms until today.

The power of molecular modelling and simulation gave rise to physically based equations of state, which Johann Fischer has pursued over two decades. He has refined the Boublík-Alder-Chen-Kreglewski (BACK) family of equations of state [8], where the various types of physical interactions are explicitly considered. He applied equations of state of this type to many engineering related systems with great success.

Johann Fischer's second relocation to Wien was associated with a transition to more energy oriented technological activities. Here, equations of state play a crucial role. Of particular mention are his accomplishments on the organic Rankine cycle to convert heat to work. His most recent seminal theoretical publications about the selection of working fluids for this process are among the top cited in this field [9,10].

As Johann Fischer's students, we very much enjoyed his thoughtfulness and patience while dedicating himself to work with us finding solutions to intricate problems. The blend of his origins in teaching and his expertise in science lead to a perfect learning environment and student–teacher relationship. We recall going with him through stacks of dot matrix printer paper containing running averages of molecular simulation results. Johann Fischer taught us the key of careful scientific work by meticulously examining data in search of gems and glitches. The sharp point of his pencil was always in motion. Many of his close collaborators will remember his many pages of output that were collages of golf-ball typewriter text, handwritten notes and sketches glued together in A4 format. Today, he has managed to transfer much of this style to emails.

Johann Fischer's 14 doctoral students and numerous other group members and collaborators extensively discussed a wide variety of topics beyond their scientific endeavours under his auspices, with history and politics being prominent among them. The knowledgeable and open minded atmosphere Johann Fischer created was inspiring to many, whether they be locals or visitors from abroad. He freely shares his scientific world view with visitors, colleagues and students from many corners of the globe with open arms, regardless of their academic status. His hospitality and generosity is regarded with deep

appreciation and is reflected by the body of work collected in this Special Issue.

The Editors and Advisory Board of *Molecular Physics* (and, in particular, George Jackson as Chair of Editors) are very grateful to Professor Fischer for his seminal and lasting contributions to the journal. We are delighted to introduce this Special Issue of *Molecular Physics* in honour of Professor Fischer, celebrating his achievements and contributions which are amply apparent from the short list of references in the bibliography (many of which were published in *Molecular Physics*). The latest contributions by his collaborators, friends and colleagues collected in this issue are but a small testament of the highest regard and esteem in which Professor Fischer is held. Deeply thankful for his guidance, we wish Johann Fischer fruitful and good times ahead.

Disclosure statement

No potential conflict of interest was reported by the authors.

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