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EDITORIAL



Editorial – special issue in honour of Peter A. Schwerdtfeger on the occasion of his 70th birthday

It is a particular pleasure for us to introduce this Special Issue of *Molecular Physics*, prepared in honour of **Distinguished Professor Peter A. Schwerdtfeger** on the occasion of his 70th birthday. For both of us, this celebration carries a deeply personal dimension: We both worked with Peter during formative years of our career and stayed in touch throughout – on a professional as well as a personal level. Editing this collection therefore felt less like a formal editorial task and more like an opportunity to reflect on the intellectual curiosity, generosity, and critical sharpness that Peter has shared so freely with his students and colleagues over decades.

Born in Stuttgart in 1955, Peter's academic path has taken him from Germany to New Zealand and on to a truly international presence in the chemical sciences – and beyond! After early training as a chemical – technical assistant and in chemical engineering, he studied chemistry, physics, and mathematics at the University of Stuttgart, where he completed his doctorate in theoretical chemistry in 1986 under Prof. Heinz Werner Preuss focusing on the development of pseudopotentials. He subsequently obtained his habilitation at University of Marburg in 1995 already living and working in New Zealand. A Feodor – Lynen fellowship of the Alexander von Humboldt (AvH) Foundation had first brought Peter to New Zealand in 1987, to the University of Auckland. He stayed strongly connected to the Foundation over a long period of his career, for example by being the president of the New Zealand and Australian AvH society. R.T.-Z. benefitted from these activities by conducting his postdoctoral stay with Peter via the very same fellowship.

After a period as a research fellow at the Australian National University in Sydney/Australia, Peter returned to Auckland, where he rose through the ranks to become Full Professor. In 2004 he was appointed to the Chair in Theoretical Chemistry at Massey University, Albany (Auckland), where he founded and directs the Centre for Theoretical Chemistry and Physics (CTCP) and serves as Head of the New Zealand Institute for Advanced Study (NZIAS). Not only has his group seen the graduation of numerous PhD students and the scientific growth of many, many postdocs, but Peter also upholds an unwavering 'open door' policy for international visitors of all

career stages, thereby creating a highly stimulating environment, and a perpetually growing network of scientific collaboration and interaction.

Peter's research activities span an impressive range, driven by his endless scientific curiosity: relativistic electronic-structure theory, the chemistry and physics of heavy elements, fundamental symmetry violations in molecules, the topology and properties of fullerenes, the origin of life, nanoclusters, close-packing of solid-state systems, phase transitions and many more topics. His work has contributed significantly to our understanding of why heavy elements behave as they do: From explaining striking phenomena such as the colour of gold and the liquid state of mercury, to setting quantitative benchmarks for weak interactions and cohesive energies in solids.

The impact of this scientific programme is reflected in numerous distinctions, including the Rutherford Medal, New Zealand's highest science honour, as well as the Humboldt Research Award, the Fukui Medal, and the Hector Medal, among many others. He was elected to the International Academy of Quantum Molecular Science (IAQMS) in 2012 and has authored several hundred publications that have shaped modern theoretical and computational chemistry.

Equally important to us as guest editors is Peter's role as a mentor and scientific role model. Both of us have had the formative experience of training and working in his group. One of us (R.T.-Z.) joined Peter's group at Massey University as a postdoctoral researcher from 2008–10, and is now Professor of Theoretical Chemistry at Leipzig University. The other (A.H.) completed his doctoral studies with Peter at Massey University between 2005 and 2009 and has since become a Professor of Computational Physics at the University of Edinburgh. Our own trajectories – in theoretical chemistry and in computational physics – reflect but some of Peter's scientific interests and his style of approaching scientific questions inspires us to this day.

Peter's mentorship style combines a sharp critical sense with a genuine enthusiasm for the subject and for the people doing it. Discussions with him are typically intense and wide-ranging: a careful dissection of

approximations and numerical details is likely to be followed by a sudden leap to broader conceptual or even philosophical questions. Many of his former students and postdocs will recognise the experience of leaving his office or group meetings with longer reading lists, new collaborations, and perhaps a fresh problem that one “might as well try” because it is interesting. The number of successful careers that trace their roots to his group in New Zealand is itself a testament to his generosity with ideas and time.

The contributions collected in this Special Issue reflect the breadth of Peter Schwerdtfeger’s scientific influence: Several articles address relativistic quantum chemistry and heavy-element systems, including studies of parity-violation sensitivity in chiral platinum complexes, relativistic effects in uranium – phosphorus bonding, Mössbauer parameters of iridium, and high-level thermochemistry of superheavy-element fluorides. Fundamental aspects of chemical bonding and electronic structure are explored in work on small molecules and clusters, magnetic response and coupling phenomena, delocalisation measures in quantum systems, and parametrizations of the homogeneous electron gas. Methodological developments included range from spinor-based coupled-cluster theory and CCSD(T)-quality adsorption energies on surfaces to first-principles treatments of surface fluorination and hydration free energies of lanthanide and actinide ions. Together, these contributions span molecules, clusters, and surfaces, and illustrate how advances in theory, methodology, and computation continue to push the frontiers of molecular physics in directions closely aligned with Peter’s long-standing scientific interests.

We are particularly pleased that this Issue brings together colleagues, collaborators, former students and postdocs, and scientific friends from across the world.

Their contributions not only highlight current frontiers in their respective fields but also form a scientific portrait of Peter’s influence across subfields and generations. In this way, the Special Issue serves at once as a tribute and as a snapshot of a vibrant research area that he significantly contributed to shape.

We would like to thank all authors and referees for their generous efforts in making this Special Issue possible, and the editorial staff of *Molecular Physics* for their support throughout the process. Above all, we thank Peter: for the science, for the mentorship, and for the friendship. It is a privilege to dedicate this collection of articles to him on the occasion of his 70th birthday, and we look forward to many more stimulating discussions and collaborations in the years to come.

Happy Birthday, Peter!

Disclosure statement

No potential conflict of interest was reported by the authors.

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