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Festschrift for Wolfgang E. Ernst – electronic and nuclear dynamics and their interplay in molecules, clusters and on surfaces

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This themed issue in *Physical Chemistry Chemical Physics* is dedicated to Professor Wolfgang E. Ernst, our dear colleague, mentor and friend, on the occasion of his 70th birthday. The title chosen reflects his broad interest in the atomistic structure of matter, its physical, optical and chemical properties, and the numerous techniques cleverly devised to interact with these systems and to manipulate their features in a controlled way. A statement commonly found in memoirs, contrasting the 'lightheartedness' of earlier years with a much more 'solid' attitude in later life, does indeed also apply to Wolfgang: literally, his research interests span from an early focus on molecular spectroscopy in the gas phase to a later taste for problems of solid-state physics, such as phase transitions in mixed-metallic compounds or electron–phonon interactions in topological insulators or semimetals. On his journey through about 5 decades of active and yet ongoing research he has been accompanied by many generations of scientists. This issue comprises more than 30 papers, authored by his former students, post-doctoral researchers, his scientific colleagues and friends, to celebrate Wolfgang's birthday.

Wolfgang was born on May 31, 1951 in Minden, Germany, and studied physics and mathematics at the Technische Universität Hannover from 1969 to 1977. Having received a scholarship from the German Academic Scholarship Foundation (Studienstiftung) in 1970, he then studied at the Imperial College London in 1972/73 and completed his diploma in physics at the University of Hanover in 1975. Only two years later, supported by the Studienstiftung, he submitted his PhD thesis (Fig. 1).

From 1978 to 1979 he worked as a post-doctoral fellow on the development of excimer lasers with Frank K. Tittel at Rice University in Houston, Texas.[1] From 1979 to 1985 he held a university assistant position at the Freie Universität Berlin, where he habilitated in 1983 in experimental physics. Wolfgang's early research was driven by the desire to explore the structure of atoms and diatomic molecules with the highest resolution and precision possible. From 1985 to 1989, a Heisenberg grant allowed him to continue as head of the Laser Laboratory for Molecular Spectroscopy at the Free University of Berlin. Research achievements from this period include the development of a laser–microwave double-resonance technique for ultra-high precision spectroscopy on molecular beams,[2] for which he was awarded the Physik-Preis of the German Physical Society in 1987. During a research year with Richard N. Zare at Stanford University, Wolfgang pioneered the application of table-top laser sources in the extreme vacuum ultraviolet regime below 100 nm, allowing him to directly access Rydberg states of atomic and molecular systems.[3]

In 1990, he accepted a tenured full professorship of physics at the Pennsylvania State University in State College, PA, where his research interests concentrated on the exploration of metal trimers and their complex interplay of rovibronic excitations, pseudorotational effects and hyperfine interactions.[4] In 1997 he was also appointed Professor of Chemistry. During his 12 years at the Pennsylvania State University, Wolfgang spent sabbaticals with Udo Buck at the Max Planck Institute for Fluid Dynamics in Göttingen (1993) and with Giacinto Scoles at Princeton University (1996), where he first delved into the field of superfluid helium nanodroplets, his primary topic of research for many years to come.

In 2001, he accepted a call to Graz University of Technology, where he headed the Institute for Experimental Physics from 2003 until his retirement in autumn 2019. In Graz, Wolfgang's research activities fully unfolded: initially, experimental techniques including

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Fig. 1 Wolfgang receiving the first flashes of inspiration for his scientific career: PhD celebration at the Technische Universität Hannover, 1977.

laser circular dichroism and magnetic resonance spectroscopy were developed to study magnetic properties of dopants in He droplets at cryogenic temperatures.[5–7] As a complementary technique, his group started to apply matter waves to explore the structure and processes of surfaces *via* elastic and inelastic helium atom scattering, and had its fingers on the pulse of time, revealing new insights on the Boson peak in amorphous materials and laying the foundation for future work on electron–phonon couplings at topological materials.[8] In parallel to these contributions to the community of solid state physics, he began to exploit the He droplet beam technique also for the growth of large metallic clusters and nanostructures, eventually adapting and perfecting it for the synthesis and non-destructive deposition of mixed-metallic nanoparticles of varying morphology, such as Janus-type or core-shell structures.[9] At first, questions regarding phase transitions and diffusion in metallic nanostructures were addressed, and the mystery of 'pearl chain'-like structures of solid metals after their He-droplet-mediated placement on supports at room temperature was lifted by the confirmation of post-deposition surface diffusion processes known as Rayleigh instabilities.[10] In later years, the focus shifted towards the usage of certain metallic combinations for optical or chemical applications as catalysts or tuned plasmon resonators. More recently, time-domain techniques in gas- and condensed phases have been added to the experimental repertoire[11,12] and become the dominating approach performed at his former institute in Graz, where new generations are aiming for a seamless continuation of his pioneering work at the interface of molecular, cluster and surface science.

This Festschrift is mostly dedicated to Wolfgang's activities during his time in Austria. It holds a diverse collection of recent studies on electronic and nuclear features of molecular systems, metallic clusters, quantum liquids and new types of matter, their atomic structure and dynamics, interplay and coupling mechanisms. Articles on a plethora of experimental techniques, from high-resolution frequency-domain studies over femtosecond time-resolved studies, to helium atom scattering, mixed with theoretical work on non-Born-Oppenheimer-effects, electronic structure calculations, molecular dynamics simulations and machine learning applications for reaction modelling. The range of probing techniques used by the authors, spanning from single- and multiphoton excitation, diffraction of electrons and atoms, to tunnelling microscopy, is equally diverse as the systems under investigation, reaching from small radicals and organic dyes in isolation, over pure and doped He droplets, to molecules in solvation and on surfaces. The scope is as broad as the research activities of Wolfgang and therefore reflects his attitude to always enter new avenues and scientific adventures.

We thank all contributing authors for their time and the energy they dedicated to these articles. Together, they have created an exceptionally rich and highly topical kaleidoscope of current research in the field. We further thank the editors of *Physical Chemistry Chemical Physics*, Catherine Au and Isobel Tibbetts, for their support and their generous efforts during the whole process of publication.

References

1 W. E. Ernst and F. K. Tittel, *Appl. Phys. Lett.*, 1979, **35**, 36–37.
2 W. E. Ernst, S. Kindt and T. Törring, *Phys. Rev. Lett.*, 1983, **51**, 979–981.
3 W. E. Ernst, T. P. Softley and R. N. Zare, *Phys. Rev. A: At., Mol., Opt. Phys.*, 1988, **37**, 4172–4183.
4 W. E. Ernst and S. Rakowsky, *Phys. Rev. Lett.*, 1995, **74**, 58–61.
5 J. Nagl, G. Auböck, C. Callegari and W. E. Ernst, *Phys. Rev. Lett.*, 2007, **98**, 075301.
6 M. Koch, G. Auböck, C. Callegari and W. E. Ernst, *Phys. Rev. Lett.*, 2009, **103**, 035302.
7 C. Callegari and W. E. Ernst, Helium Droplets as Nanocryostats for Molecular Spectroscopy – from the Vacuum Ultraviolet to the Microwave Regime, *Handbook of High Resolution Spectroscopy*, John Wiley & Sons, Chichester, 2011.
8 W. Steurer, A. Apfolter, M. Koch, W. E. Ernst, B. Holst, E. Sondergad and J. R. Manson, *Phys. Rev. Lett.*, 2007, **99**, 035503.
9 W. E. Ernst and A. W. Hauser, *Phys. Chem. Chem. Phys.*, 2021, **23**, 7553–7574.

10 A. Volk, P. Thaler, D. Knez, A. W. Hauser, J. Steurer, W. Grogger, F. Hofer and W. E. Ernst, *Phys. Chem. Chem. Phys.*, 2016, **18**, 1451–1459.

11 P. Heim, S. Mai, B. Thaler, S. Cesnik, D. Avagliano, D. Bella-Velidou, W. E. Ernst, L. González and M. Koch, *J. Phys. Chem. Lett.*, 2020, **11**, 1443–1449.

12 B. Thaler, S. Ranftl, P. Heim, S. Cesnik, L. Treiber, R. Meyer, A. W. Hauser, W. E. Ernst and M. Koch, *Nat. Commun.*, 2018, **9**, 4006.