A Personal Preface to the Special Issue of Molecular Physics in Honour of Professor Timothy P. Softley, FRS

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The following collection of 25 papers have been submitted in honour of Professor Tim Softley, FRS to mark his 60th birthday. These papers tell us much about the man honoured in this special issue. They have been authored by chemists, physicists, experimentalists and theoreticians alike from many countries on three continents. The subject matter ranges from individual atoms *via* diatomic and small molecules to fluorescent protein chromophores and from electron transfer in nucleobase clusters to matter-wave interferometry.

It is with great pleasure and a feeling of gratefulness that we - the first three graduate students to benefit from Tim's inspirational supervision - present the following brief outline of his scientific career. A short curriculum vitae and publications list follows.

Born in Norwich, England in 1958, Tim was state-school educated and passed the entrance exam to matriculate at Wadham College in Oxford in 1977, graduating with a 1st class Chemistry BA degree in 1981. Tim then headed for better climes – firstly to the English Riviera for his PhD in Southampton with Alan Carrington and then to Stanford, California for postdoctoral research with Richard Zare. He returned to the UK on a research fellowship in Cambridge before his appointment as University Lecturer (later Reader, then Professor of Chemical Physics) in Physical Chemistry in Oxford in association with Merton College. After 25 years in Oxford, in 2015 he then took up his present post as Pro Vice Chancellor for Research and Knowledge Transfer at the University of Birmingham, the UK's largest University.

Tim has authored or co-authored over a hundred papers with more than 160 co-authors. His publication list is appended to the curriculum vitae which follows this preface and covers a broad range of topics in molecular physics, including high-resolution spectroscopy, reaction dynamics and cold chemistry. His research is characterised by a passion for the development of original instrumentation and measurement techniques – he is not a scientist who found his niche and settled therein but rather one driven by curiosity and the desire to understand matter at the atomic and molecular level. When visiting his laboratory in Oxford, one cannot help admiring the astonishing range and diversity of experimental facilities he has developed over his career: Narrow band VUV lasers for photoionization and photoelectron spectroscopy, Stark and Zeeman decelerators for the production of cold atoms and molecules, complex vacuum systems hosting Coulomb crystals for the study of low-temperature ion-molecule reactions, and much more.

From the complexity of the instruments, one first concludes that Tim's scientific activity is that of a pure experimentalist. Those who worked closely with him know better: For Tim, building new, more performant instruments is not a goal per se, but the best way to stimulate theoretical or modelling activity: A good experimentalist is not a scientist capable of doing good experiments but one who is forced to do good experiments by an internal need to clarify his or her own theoretical understanding. "A good experiment forces you to think correctly about the problem you are studying" he would tell his coworkers. It is this aspect of Tim's scientific activity which made it so attractive to work under his supervision.

Tim's independent research, began in Cambridge in the late 1980s, and involved the development of narrowband tuneable VUV radiation for high-resolution photoelectron spectroscopy of atoms and small molecules. Around this time, the new technique of zero-kinetic-energy (ZEKE) photoelectron spectroscopy, based on field ionization of high–lying Rydberg states was emerging. The Softley group played an important role in understanding channel interactions in atomic and small molecular systems and modelling these interactions with multichannel quantum defect theory. Typical of Tim's flexible thinking, he saw the possibility of using the field ionization of high Rydberg states to prepare molecular cations in specific ro–vibrational states and to study the rotational-state dependence of ion-molecule reactions.

The late 1990s and early 2000s saw threshold photodissociation studies, including some early velocity-map-imaging studies, as well as Tim's first foray into the manipulation of neutral atoms and molecules using the enormous dipole moments achieved in excitation of high-n Rydberg states. This was to become a theme in subsequent research with both the Stark and Zeeman effects later being employed to guide cold samples of state–selected molecules. Since then, major new research efforts have been devoted to studying interactions of Rydberg atoms and

molecules with metallic surfaces, and performing innovative cold-chemistry experiments combining Ca^+ Coulomb crystals with cold molecular beams.

Tim also excels in University leadership roles. He was a very young Senior Proctor of Oxford University in 2002/3, responsible for enforcing University discipline and sanctions and handling complaints, along with briefing Her Majesty the Queen on the latest developments within the University. This was followed by a stint as sub-warden of Merton College, a notoriously challenging task *akin* to herding cats. These roles prepared him well for subsequent positions as Associate Head of Division in Oxford (2006–2011), Head of Physical and Theoretical Chemistry (2010–11) and then Chairman of Chemistry and Head of Department (2011–2015). Leading a department of over 80 research groups in turn prepared him well for his current activity as Pro Vice Chancellor at the University of Birmingham.

However, it is Tim's science that we celebrate here and *Molecular Physics* could not be a more natural home: Tim served tirelessly on the Editorial Board of *Molecular Physics* from 1999 to 2004 and then as Chair of the Editors from 2004 to 2016, a time during which he launched multiple initiatives to ensure the prosperity of the journal.

April 2019 saw a two-day scientific symposium *New Horizons of Chemical Physics* in Oxford which served to mark Tim's 60th birthday (see Figure 1). All speakers had a close scientific relationship with Tim, from his postdoc supervisor, Dick Zare, to long-term collaborators including Michael Drewsen, Heather Lewandowski, Matthias Keller and Katharine Reid. Ex-Softley-group members Katrin Dulitz, Oliver Monti, Elin McCormack, Andrew Hudson, David Townsend, Stefan Willitsch and Brianna Heazlewood completed the scientific programme.

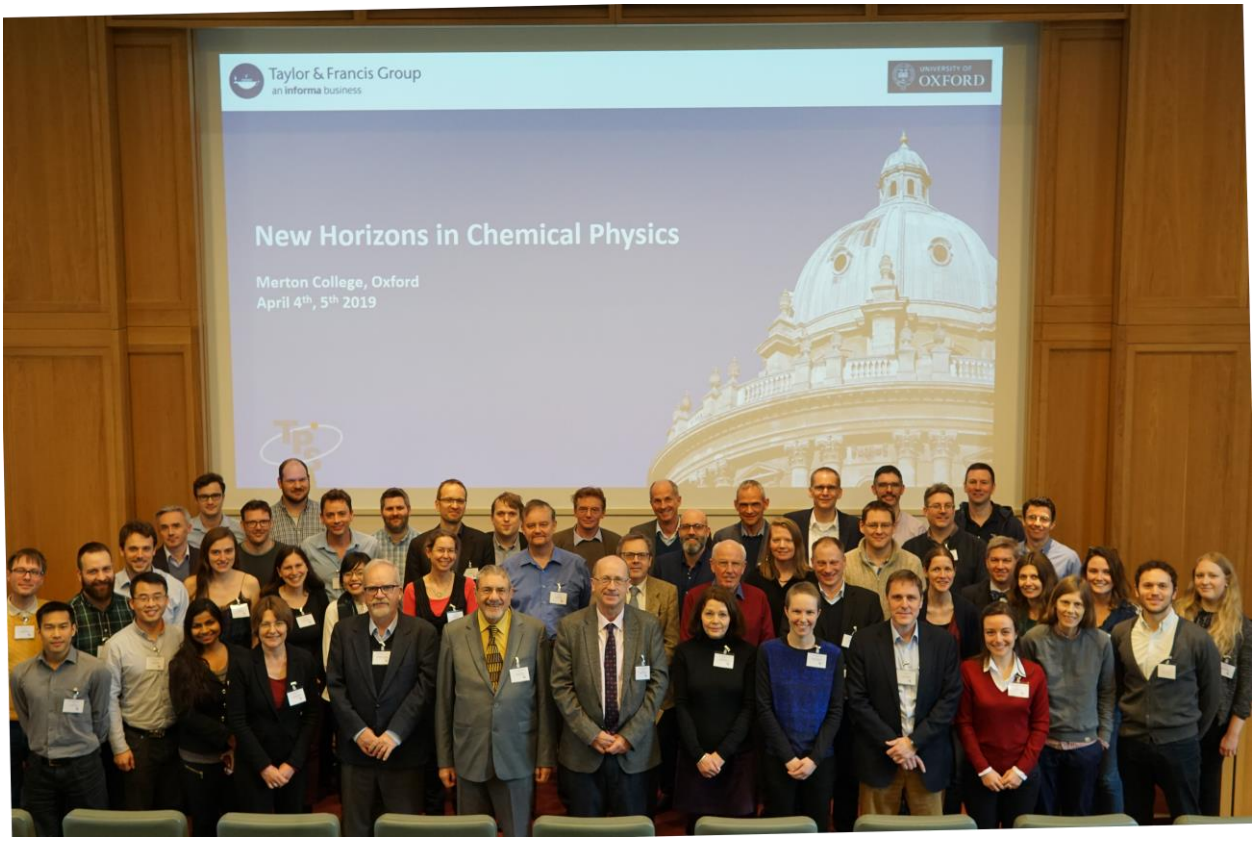

Figure 1: Conference photo from the New Horizons in Chemical Physics meeting in Oxford, April 4th, 5th 2019 held to celebrate Tim Softley's 60th birthday.

Over the years, Tim has supervised more than 30 PhD students and a similar number of postdoctoral fellows. If we were to interpret the way he led his research group, we could summarize it as follows: Give your co-workers interesting scientific problems to work on, let them work at their own pace, inspire them by example, foster scholarship, maintain an open research climate and an intellectually stimulating atmosphere. His co-workers gratefully remember the wonderful Christmas dinners at his and Tertia's home, and the discussions in his office, during which it was not uncommon to witness multiple pages being filled with 3j symbols, angular-momentum coupling schemes, and schematic experimental diagrams. Tim has

always been an extremely encouraging and supportive supervisor and many of us can remember the first conversation with Tim in which he encouraged us to think positively, often for the first time, about the next steps in our careers.

Beyond science, Tim has a passion for tennis, singing (including with the celebrated Oxford Bach choir) and hiking. By location of his birth, Tim was cursed to support Norwich City football club – a classic yo-yo team, which, during Tim's life has been promoted and relegated in equal number (eight each), their one highlight coming in a 2-1 victory against Bayern Munich in the Olympiastadion in the UEFA cup 2nd round 1993.

As guest editors for this special issue, we are grateful to the very many people who have contributed as authors or reviewers, and, of course, to Tim for being the source of inspiration and motivation.

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