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THERMODYNAMICS 2017

Thermodynamics 2017 Conference — Edinburgh, Scotland, 5–8 September 2017

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Thermodynamics is a cornerstone of the scientific and engineering disciplines encompassing core branches of chemistry, physics, biology, chemical engineering, petroleum engineering, and materials science. The thermodynamic interrelationships between heat, work, and energy are the basis for understanding the properties of matter and its transformations, which are at the heart of the design and optimisation of industrial processes, and the development of advanced materials and products. Thermodynamics provides a platform from which scientists and engineers can analyse and describe complex systems from the microscopic (molecular) level to the macroscopic scale of bulk matter. Although its origins date back to the scientific revolution, thermodynamics has continued to evolve, benefitting from advances in experimental techniques, theoretical formalism, and numerical molecular simulation. As a consequence of some of the more recent developments, the discipline is becoming relevant to an increasing number of domains including the complex supramolecular arrangements ubiquitous in the life sciences, nano-materials and colloidal systems in which short-range interactions can be dominant, and complex fluids such as liquid crystals, polyelectrolytes, and ionic liquids, which have been the subject of much current attention.

The *Thermodynamics 2017 Conference* was the 25th meeting in a series of biennial thermodynamics conferences conceived in the 1960s by Sir John Rowlinson and Max McGlashan, and initiated in Keele by Harold Springall (Spring as he was affectionately known by his friends including Linus Pauling). Although the original emphasis of the science presented at the meetings was on experimental thermodynamics, the *Thermodynamic Conference Series* (TCS) now has a wide remit encompassing broad areas of the discipline including experiment, theory, and molecular simulation. The meetings were traditionally held in the UK (see Table 1) until 2005 when the conference was hosted by Eduardo Filipe and José Nuno Canongia Lopes in Sesimbra, a picturesque fishing village 40 km from Lisbon. In view of the great success of the Portuguese conference, it was decided to hold TCS meetings in both the UK and continental Europe from then on. In 2017, the conference was held in Edinburgh, Scotland (see Figure 1).

After the faithful, selfless and single-handed stewardship of Christopher Wormald in the 1990s, the TCS began its close association with the *Statistical Mechanics and Thermodynamics Group* (SMTG) of the Faraday Division of the Royal Society of Chemistry (RSC). As an independent organisation, the remit of the TCS is the promotion of thermodynamics as a scientific discipline, to improve its techniques, and to advance their application in science and technology through the organisation of biennial conferences, bringing together researchers from academia and industry from all over the world. The TCS is managed by a permanent Steering Committee, at present comprising the Treasurer of the Conference Series (who acts as the Presiding Officer of the Committee), the Chair of the SMTG Management Committee, an additional member of the SMTG, a UK-based member, the acting *Thermodynamics Conference* Chair, the immediate past *Thermodynamics Conference* Chair, and members of the International Scientific and the Local Organizing Committees. The constitution of the TCS Steering Committee for the *Thermodynamics 2017 Conference* and the forthcoming *Thermodynamics 2019 Conference* which is to be held in Huelva (Spain) is shown in Table 2.

Three prizes are currently awarded at the *Thermodynamics Conferences*: the *Lennard-Jones Lectureship and Prize* in recognition of outstanding and enduring contributions to the field of statistical mechanics and thermodynamics (see Table 3); the *Guggenheim Medal for Excellence in Thermodynamics*, awarded by the Institution of

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Table 1. *Thermodynamic Conference Series*: the Presiding Officer of the TCS Steering Committee is indicated in brackets.

	Year	Conference Venue	Conference Chairs
1	1964	Keele	H. D. Springall
2	1966	Exeter	M. L. McGlashan
3	1968	Manchester	H. A. Skinner
4	1970	Surrey (Royal Holloway)	J. S. Rowlinson
5	1972	Lancaster	M. L. McGlashan
6	1974	Leeds	L. A. K. Staveley
7	1976	Bristol	J. D. Cox
8	1978	Surrey	J. D. Cox
9	1980	London (University College)	G. Pilcher
10	1984	Sheffield	I. A. McLure & C. J. Wormald
11	1986	Reading	M. B. Ewing
12	1988	Leicester	R. G. Linford
13	1993	Bristol	C. J. Wormald
14	1995	Reading	C. J. Wormald
15	1997	Surrey	C. J. Wormald
16	1999	London (Imperial College)	C. J. Wormald
17	2001	Bristol	M. P. Allen (J. P. M. Trusler)
18	2003	Cambridge	A. A. Louis (J. P. M. Trusler)
19	2005	Sesimbra	E. Filipe & J.N. Canongia Lopes (J. P. M. Trusler)
20	2007	Paris (Institut Français du Pétrole)	J.-C. de Hemptinne (G. Jackson)
21	2009	London (Imperial College)	E. A. Müller (G. Jackson)
22	2011	Athens	I. G. Economou (G. Jackson)
23	2013	Manchester	A. J. Masters (G. Jackson)
24	2015	Copenhagen	G. Kontogeorgis & E. H. Stenby (G. Jackson)
25	2017	Edinburgh	L. Sarkisov & M. B. Sweatman (G. Jackson)

Figure 1. *Thermodynamics 2017 Conference* photo.

Chemical Engineers (IChemE) for the first time in 2015 (see Table 4), and the *Christopher Wormald Prize* awarded to the most meritorious postgraduate research at the TCS as nominated by members of the community (see Table 5). *The Lennard-Jones Lectureship and Prize* has a long and illustrious history; it was originally awarded in alternate years by the *Theoretical Chemistry Group* (TCG) and the SMTG of the RSC, then biennially by the SMTG alone; since 2001 it has been presented at the TCS. Nominations for the *Lennard-Jones Lectureship and Prize* are made by the SMTG Management Committee to the TCS during the organisation of the programme for the *Thermodynamics Conference*, at which the recipient of the prize gives a keynote presentation. The 2017 *Lennard Jones Lectuership and Prize* was awarded to Ruth Lynden-Bell (see Figure 2), the 2017 *Guggenheim Medal* was jointly awarded to Pablo Debenedetti (see Figure 3) and to Martin Trusler (see Figure 4), and the 2017 Wormald Prize was awarded to Rachael Mansbach (see Figure 5). A keynote *Molecular Physics Lecture* sponsored by Taylor and Francis Ltd is also one of the crowning features of the TCS (see Table 6 for past lecturers). Carlos Vega was chosen as the *Molecular Physics Lecturer* for the *Thermodynamics 2017 Conference*; he was unfortunately

Table 2. Membership of the TCS Steering Committee.

Role	Thermodynamics 2017	Thermodynamics 2019	Tenure/ years
Treasurer of TCS (and Presiding Officer)	G. Jackson	A. Galindo	8
Chair of SMTG	K. P. Travis	K. P. Travis	4
Member of SMTG	A. Galindo	F. Bresme	2
UK-based member	S. Brandani	G. Jackson	2
Acting Chair of *Thermodynamics Conference*	L. Sarkisov M. Sweatman	F.J. Blas	2
Immediate Past Chair of *Thermodynamics Conference*	G. Kontogeorgis E. H. Stenby	L. Sarkisov M. Sweatman	2
Members of the International Scientific Committee	M. Anismov S. Little A. J. Masters V. Milman M. Noro P. Pullumbi C. Vega T.Vlugt	J. Coutinho P. T. Cummings I. Economou A. Gil-Villegas K. E. Gubbins P. Paricaud	2
Members of the Local Organizing Committee	A. Farmahini M.-C. Ferrari G. Santori C. McIlwraith	A. Cuetos Menéndez P. Gómez Álvarez L. González MacDowell E. González Noya J. Largo Maeso E. Lomba García M. Martínez Piñeiro J. M. Míguez Díaz J. M. Romero-Enrique	2

Table 3. *Lennard-Jones Lectureship and Prize* in recognition of outstanding and enduring contributions to the field.

Year	Recipient	Awarded by
1982	J. A. Pople	SMTG / TCG Joint
1983	L. A. K. Staveley	SMTG
1984	N. C. Handy	TCG
1985	J. S. Rowlinson	SMTG
1986	A. D. Buckingham	TCG
1987	J. M. Deutch & I. Oppenheim	SMTG
1988	G. G. Hall	TCG
1989	P.-G. de Gennes	SMTG
1990	A. J. Stone	TCG
1991	W. M. Gelbart	SMTG
1992	B. T. Sutcliffe	TCG
1993	B. Widom	SMTG
1995	M. E. Fisher	SMTG
1997	D. Frenkel	SMTG
1999	E. Sackmann	SMTG
2001	D. Chandler	SMTG
2003	J.-P. Hansen	SMTG
2005	G. Schneider	SMTG
2007	R. Evans	SMTG
2009	K. Binder	SMTG
2011	H. N. W. Lekkerkerker	SMTG
2013	K. E. Gubbins	SMTG
2015	M. P. Allen	SMTG
2017	R. M. Lynden-Bell	SMTG

Table 4. *Guggenheim Medal* for excellence in thermodynamics.

Year	Recipient	Awarded by
2015	G. Jackson	IChemE
2017	P. Debenedetti & J. P. M. Trusler	IChemE

indisposed and his friend and collaborator Eduardo Sanz kindly delivered the lecture on some of their joint work (see Figure 6).

Table 5. *Christopher Wormald Prize* for most meritorious postgraduate research.

Year	Recipient	Awarded by
2003	R. Allen	TCS
2005	J. Lachwa	TCS
2007	T. Lafitte & E. E. Santiso	TCS
2009	F. Martínez-Veracoechea	TCS
2011	A. S. Avlund	TCS
2013	E. Forte	TCS
2015	N. Mahynski	TCS
2017	R. Mansbach	TCS

The *Thermodynamics 2017 Conference* was held in Edinburgh, Scotland between the 5th and 8th of September 2017, and was attended by about 180 academic and industrial participants from 30 countries. The science presented at the meeting included the following broad themes: statistical mechanics and equations of state; novel experimental methods; molecular modelling and simulation; multi-scale modelling from quantum mechanics to engineering approaches; transport properties of complex fluids; interfacial phenomena; polymers and other materials; ionic liquids and green processes including supercritical fluids; aqueous systems and electrolytes; pharmaceuticals; nano-scale processes; carbon dioxide and conventional energy production.

The format of the conference consisted of invited plenary lectures, oral presentations, and posters. The highlights of the *Thermodynamics 2017 Conference* included: the *Lennard-Jones Lecture* by Ruth Lynden-Bell entitled 'Atomistic simulation – a molecular scale view of solutions' (sponsored by Unilever); the *Molecular*

Figure 2. Recipient of *Lennard-Jones Lectureship and Prize*: Ruth Lynden-Bell (presented by Karl Travis, Chair of the SMTG)

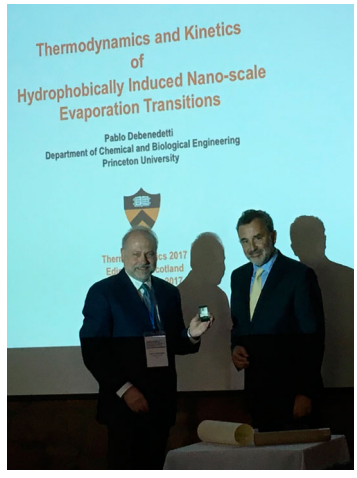

Figure 3. Joint Recipient of *Guggenheim Medal* for excellence in thermodynamics: Pablo Debenedetti (presented by Ioannis Economou, Chair of the IChemE *Guggenheim Medal* Panel).

Figure 4. Joint Recipient of *Guggenheim Medal* for excellence in thermodynamics: Martin Trusler (presented by Ioannis Economou, Chair of the IChemE *Guggenheim Medal* Panel).

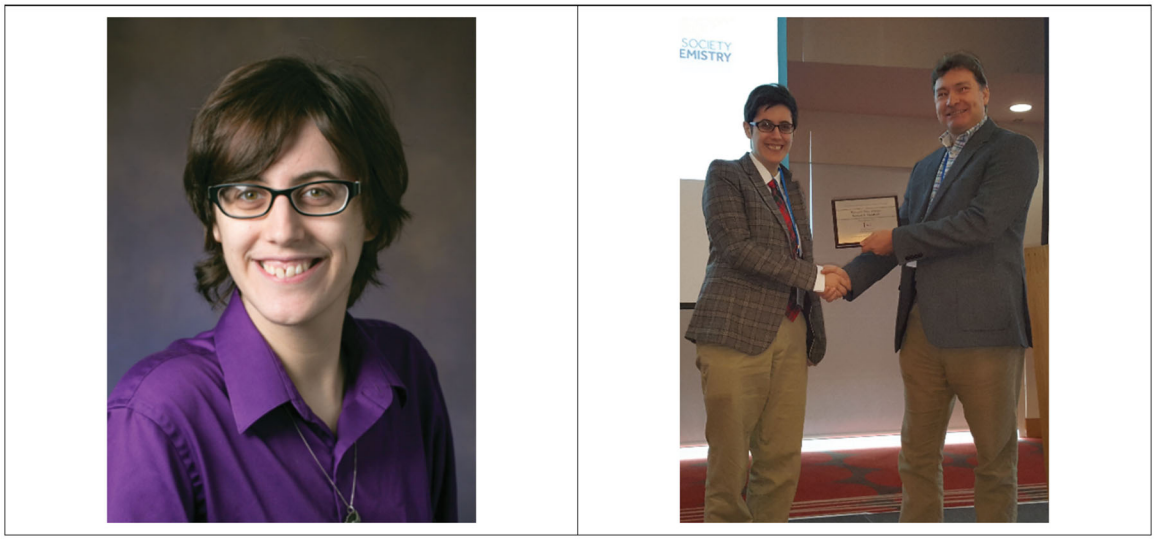

Figure 5. Recipient of *Christopher Wormald Prize* for most meritorious postgraduate research: Rachael Mansbach (presented by Martin Sweatman, Co-Chair of the *Thermodynamics 2017 Conference*).

Table 6. The *Molecular Physics Lectures.*

Year	Lecturer	Title
2009	K. E. Gubbins	*The theory of non-electrolyte solutions: a recent history.*
2011	W. L. Jorgensen	*Accelerated drug discovery through computer simulations of protein-inhibitor complexes.*
2013	D. Frenkel	*Entropy and packing.*
2015	P. G. Debenedetti	*Thermodynamics and kinetics of deeply supercooled water: a computational perspective.*
2017	C. Vega (presented by E. Sanz)	*Seeding approach to crystal nucleation.*

Figure 6. *Molecular Physics Lecturer*: Carlos Vega (lecture delivered by Eduardo Sanz and plaque presented by George Jackson, Editor and Chair of *Molecular Physics*).

Physics Lecture presented by Eduardo Sanz on behalf of Carlos Vega entitled 'Seeding approach to crystal nucleation' (sponsored by Taylor and Francis Ltd); two separate *Guggenheim Medal* Lectures by joint recipients Pablo Debenedetti and Martin Trusler entitled 'Nanoscale drying and hydration phenomena' and 'Interfacial properties of systems comprising carbon dioxide, brine, diluent gases and minerals' respectively (awarded by the IChemE); and the presentation by Rachael Mansbach, the recipient of the *Christopher Wormald Prize*, entitled 'Multiscale molecular simulation for the study of a self-assembling optoelectronic peptide'.

The members of the TCS Steering Committee are very grateful to the editors of *Molecular Physics* for supporting

the publication of this special issue of the journal dedicated to the *Thermodynamics 2017 Conference* and to the publishers (Taylor and Francis Ltd) for sponsoring the event, as they have done since the 2007 conference. Contributions from participants are being published following review and editing to the usual high standard, as was done for the *Thermodynamics 2011 Conference* in Athens [1], the *Thermodynamics 2013 Conference* in Manchester [2], and the *Thermodynamics 2015 Conference* in Copenhagen [3]. The novel and exciting research presented at the conference will be abundantly apparent from the papers collected here. On behalf of the TCS we warmly invite you to the *Thermodynamics 2019 Conference* in Huleva, chaired by Felipe Blas (see http://www.thermodynamics2019.org for further details).

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