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Thermodynamics 2024 Conference Delft, The Netherlands 4–6 September 2024

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Figure 1. *Thermodynamics 2024 Conference* Participants gathered at Het Prinsenhof (“The Court of the Prince”) Museum in Delft.

The *Thermodynamics 2024 Conference* was the 28th meeting in this 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 *Thermodynamics Conference Series* (TCS) now has a wide remit encompassing broad areas of the discipline including

experiment, theory, molecular simulation, and machine-learning (ML) and artificial-intelligence (AI) based models. 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 2024, the conference was held for the first time Delft, a city and

Table 1. *Thermodynamics Conference Series (TCS)*; 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)
26	2019	Huelva	F. J. Blas (A. Galindo)
27	2022	Bath	C. Herdes (A. Galindo)
28	2024	Delft	O. A. Moulτος & T. J. H. Vlugt (A. Galindo)

municipality in the province of South Holland known for its historical connections with the reigning House of Orange-Nassau, for its blue pottery, and for being home to the painter Jan Vermeer. From the foundational van der Waals equation of state to the pioneering high-pressure experimental research of the groups in Delft led by Jacob de Swaan Arons, Theo de Loos, and Cor Peters, the Dutch legacy in thermodynamics continues to shape the field, fittingly celebrated here in Delft at the conference. A photograph of the participants of the *Thermodynamics 2024 Conference* is shown in 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) of the UK. As an independent organisation, the TCS is managed by a permanent Steering Committee, at present comprising the Treasurer of the TCS (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 Organising Committees. The constitution of the TCS Steering Committee for the *Thermodynamics 2024 Conference* and the forthcoming *Thermodynamics 2026 Conference*, which is to be held at Imperial College London, is shown in Table 2.

Table 2. Membership of the TCS Steering Committee.

Role	Thermodynamics 2024	Thermodynamics 2026	Tenure/years
Treasurer of TCS (and Presiding Officer)	A. Galindo	A. Galindo	8
Chair of SMTG	A. J. Masters	A. J. Masters	4
Member of SMTG	F. Bresme	F. Bresme	2
UK-based member	G. Jackson	G. Jackson	2
Acting Chair(s) of <i>Thermodynamics Conference</i>	O. A. Moulτος & T. J. H. Vlugt	E. A. Müller & J. P. M. Trusler	2
Immediate Past Chair(s) of <i>Thermodynamics Conference</i>	C. Herdes	O. A. Moulτος & T. J. H. Vlugt	2
Members of the International Scientific Committee	F. J. Blas F. Bresme P. T. Cummings I. Economou A. Galindo C. Herdes S. Kjelstrup G. Jackson	F. J. Blas P. T. Cummings I. Economou S. Enders C. Held S. Kjelstrup A. Mejía O. A. Moulτος M. Richter T. J. H. Vlugt	2
Members of the Local Organizing Committee	F. de Meyer G. Krooshof M. Mooijer A. Rahbari M. Ramdin R. Tuinier	C. S. Adjiman F. Bresme A. Galindo A. J. Haslam G. Jackson A. M. Lonergan	2

Three prizes are currently awarded at the TCS: the *Lennard-Jones Lectureship and Prize* in recognition of outstanding and enduring contributions to the field (see



Figure 2. Recipient of the 2024 *Lennard-Jones Lectureship and Prize*: Mike E. Cates (left), Lucasian Professor of Mathematics at the University of Cambridge, UK (presented by Amparo Galindo (right), representing the SMTG of the RSC).

Table 3); the *Guggenheim Medal for Excellence in Thermodynamics*, awarded by the Institution of Chemical Engineers (ICHEME, see Table 4); and the *Christopher Wormald Prize*, awarded to the most meritorious post-graduate 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 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 2024 *Lennard-Jones Lectureship and Prize* was awarded to Mike Cates (see Figure 2), the 2024 *Guggenheim Medal* was awarded to Amparo Galindo (see Figure 3), and the 2024 *Wormald Prize* was awarded to Stefanie Walter (see Figure 4). A keynote *Molecular Physics Lecture* sponsored by the publishers (Taylor & Francis Group) is also one of the crowning features of the TCS (see Table 6 for past lecturers); Tyler R. Josephson was the *Molecular Physics*

Lecturer at the *Thermodynamics 2024 Conference* (see Figure 5).

The *Thermodynamics 2024 Conference* was held in Delft, the Netherlands, between the 4th and 6th of September 2024, and was attended by about 141 academic and industrial participants from 30 countries. The 154 scientific contributions presented at the meeting included the following broad themes: statistical mechanics and equations of state; novel experimental methods; molecular modelling, simulation, and ML/AI models; 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; nanoscale processes; carbon dioxide and conventional energy production. Travel grants for two PhD students from underrepresented countries (India, Brazil) were provided thanks to the generous sponsorship from the TU Delft Pro2tech institute and the TU Delft Institute for Computational Science and Engineering. The RASPA2024 workshop, organised by David Dubbeldam, Sofia Calero, Randall Q. Snurr, Othonas A. Moulton,



Figure 3. Recipient of the 2024 Guggenheim Medal for Excellence in Thermodynamics: Amparo Galindo, Professor of Physical Chemistry at Imperial College London, UK (awarded by the IChemE).



Figure 4. Recipient of the 2024 *Christopher Wormald Prize* for most meritorious postgraduate research: Stefanie Walter (second from right), AbbVie Deutschland GmbH (presented by Thijs J. H. Vlugt (left), Othonas A. Moulτος (second from left), and George Jackson (right) representing the TCS).

Table 3. *Lennard–Jones Lectureship and Prize.*

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
2019	D. Evans	SMTG
2022	J. Yeomans	SMTG
2024	M. E. Cates	SMTG

Table 4. *Guggenheim Medal for Excellence in Thermodynamics.*

Year	Recipient	Awarded by
2015	G. Jackson	ICHEME
2017	P. Debenedetti	ICHEME
	J. P. M. Trusler	
2019	D. Theodorou	ICHEME
2022	K. A. Koh	ICHEME
2024	A. Galindo	ICHEME

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	TCS
	E. E. Santiso	
2009	F. Martínez-Veracoechea	TCS
2011	A. S. Avlund	TCS
2013	E. Forte	TCS
2015	N. Mahynski	TCS
2017	R. Mansbach	TCS
2019	J. R. Espinosa	TCS
2022	F. L. Thiemann	TCS
2024	S. Walter	TCS



Figure 5. *Molecular Physics Lecturer 2024:* Tyler R. Josephson (centre), Assistant Professor in Chemical, Biochemical, and Environmental Engineering, University of Maryland, USA (presented by Nigel Balmforth (right), Portfolio Manager, Taylor & Francis Group, and George Jackson (left), Editor and Chair of *Molecular Physics*).

Table 6. *Molecular Physics Lectures.*

Year	Lecturer	Title
2009	K. E. Gubbins	<i>The theory of non-electrolyte solutions: A recent history.</i>
2011	W. L. Jorgensen	<i>Accelerated drug discovery through computer simulations of protein-inhibitor complexes.</i>
2013	D. Frenkel	<i>Entropy and packing.</i>
2015	P. G. Debenedetti	<i>Thermodynamics and kinetics of deeply supercooled water: A computational perspective.</i>
2017	C. Vega (presented by E. Sanz)	<i>Seeding approach to crystal nucleation.</i>
2019	P. T. Cummings	<i>The molecular simulation design framework (MoSDeF): Capabilities and applications.</i>
2022	A. Gil-Villegas	<i>Quantum molecular thermodynamics.</i>
2024	T. R. Josephson	<i>Writing bug-free software using Lean.</i>

and Thijs J.H. Vlugt was also held in Delft prior to the *Thermodynamics 2024 Conference*. This workshop served as an introduction to the RASPA software for molecular simulation of nanoporous materials and fluids [1]. Randall Q. Snurr was lecturer at RASPA2024 and gave a plenary lecture at *Thermodynamics 2024*.

The format of the conference consisted of invited plenary lectures, oral presentations, and posters. The highlights of the *Thermodynamics 2024 Conference* included: the *Lennard-Jones Lecture* by Mike E. Cates entitled “Surprises in the statistical mechanics of active matter” (awarded by the SMTG and sponsored by Unilever); the *Molecular Physics Lecture* presented by Tyler R. Josephson entitled “Writing bug-free software using Lean” (sponsored by the Taylor & Francis Group); the *Guggenheim Medal Lecture* by Amparo Galindo entitled “Following Guggenheim: from conformality to molecular modelling and property prediction” (awarded and sponsored by the IChemE); and the presentation by Stefanie Walter, the recipient of the *Christopher Wormald Prize* entitled “Application of thermodynamic modelling in the design and manufacturing of pharmaceutical formulations” (awarded and sponsored by the TCS).

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 2024 Conference* in Delft. We thank the publishers (Taylor & Francis Group) for sponsoring the event, as they have done

since the 2007 conference. Contributions from participants are published following review and editing to the usual high standard of the journal, as was done for the *Thermodynamics 2011 Conference* in Athens [2], the *Thermodynamics 2013 Conference* in Manchester [3], the *Thermodynamics 2015 Conference* in Copenhagen [4], the *Thermodynamics 2017 Conference* in Edinburgh [5], the *Thermodynamics 2019 Conference* in Huelva [6], and the *Thermodynamics 2022 Conference* in Bath [7]. 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 2026 Conference* at Imperial College London, 13–15 September 2026, chaired by Erich A. Müller and J. P. Martin Trusler (see <https://thermodynamics2026.org/> and contact thermodynamics2026@imperial.ac.uk for further details).

Disclosure statement

No potential conflict of interest was reported by the author(s).

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