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Noel Sydney Hush (1924–2019)

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ABSTRACT

Noel Hush left Sydney with his MSc in 1949 to work in Manchester, and then Bristol, before returning to the University of Sydney in 1971 as the inaugural professor of theoretical chemistry, the first such chair in Australia. His students and collaborators occupy senior positions in Australian and international universities. With theoreticians and experimentalists he researched electron transfer in electrochemical changes, between metal ions, in covalent bond frameworks, in surface chemistry of gold, and in complex organic and bio-organic molecules. He was a leader among Australian academics, protesting the restrictions placed on Russian Jewish scientists who wished to leave their homeland. He was elected to fellowship of the Australian Academy of Science and the Royal Society of London, and he continued research long after the formal retirement age.

Keywords: electron transfer, organic wires, Penrose, photosynthesis, porphyrins, quantum, refuseniks, theoretical chemistry.

Introduction

Noel Sydney Hush (1924–2019) AO FAA FRS FRACI FRSN (Fig. 1) was an outstanding theoretical chemist who began and ended his long career at the University of Sydney, having held university appointments in the United Kingdom (UK) and visiting appointments at United States universities. During the seventy years that Hush was an active researcher, there was significant development of the tools available to theoretical chemists, and he was always at the forefront of those employing them. It is significant, too, that he always worked on chemical phenomena that were of interest to researchers in other branches of chemistry, drawing on their findings, stimulating their research and often collaborating with them.

Hush returned to Sydney in 1971 as foundation professor in the new department of Theoretical Chemistry. It was the first of its kind in Australia. The seeds for this had been sown much earlier, however, when Hush was a student at Sydney, where research in theoretical chemistry was being conducted under the auspices of physical chemistry. When R. D. Brown, who was just beginning his career as a theoretical chemist at the University of Melbourne (Godfrey and others 2010), visited Sydney in 1946, he met Hush and kindred spirits in David Craig (Hush and Radom 2017) and Craig's graduate student Ian Ross (Fischer and Gilbert 2009). Not just Hush, but all four went on to contribute to theoretical chemistry in Australia—Craig moving soon to University College London but later becoming professor of chemistry at the Australian National University; Ross as professor of chemistry at the Australian National University; and Brown moving from Melbourne in 1960 to be foundation professor at Monash University—but Brown later remarked that they were 'all very isolated working in Australia in those days' (Godfrey and others 2010). The field remained sparsely populated here until it developed in the 1970s and 1980s under Hush's leadership. His vision was to concentrate people to establish a national and international profile for the discipline.

As well as the bibliography of his many publications (see Supplementary Material), in compiling this biographical memoir we have drawn on other sources of information about Hush and his work.[1]

[1]The transcript of an interview with Hush conducted on behalf of the Australian Academy of Science (AAS) in 2011 is available at https://www.science.org.au/learning/general-audience/history/interviews-australian-scientists/professor-noel-hush-theoretical, viewed April 2025. Reimers (2019).

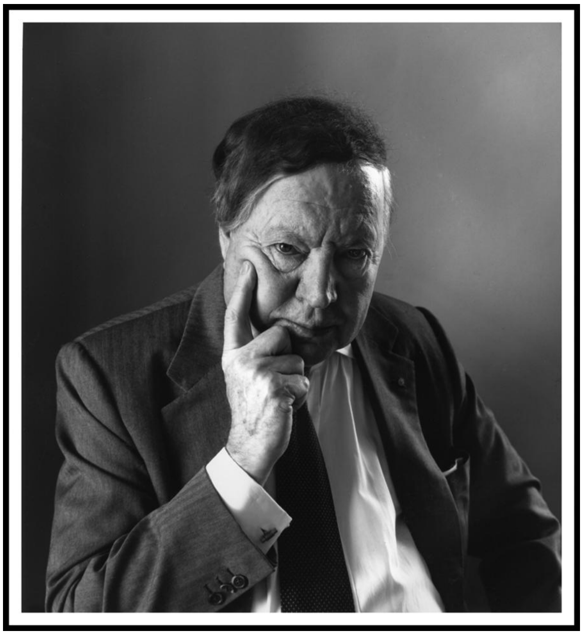

Fig. 1. Noel Hush (Philip Kuchel).

Early years

Hush was born in Sydney on 15 December 1924 to Sydney Edgar Hush, a butcher, and his wife Adrien Bessie née Cooper. Noel attended a government primary school and a private secondary school. Completing his schooling in 1941, he achieved near-perfect marks in eight subjects at the Intermediate Certificate examinations, and entered university in 1942 at age 17. From the experience of formal learning in his school and university years, augmented by prolific reading of accounts of scientific development, Hush had developed an appreciation of developments in modern physics, including quantum mechanics. Rather than being led into the study of physics, however, his stronger interest was in the application of these ideas to chemistry and the properties of chemical substances.

While he was an undergraduate at the University of Sydney, Hush was actively engaged in student politics, and he was a member of the editorial board of the student newspaper, *Honi Soit.* Following a controversy over the paper's publication of an issue in which religious and sexual views were attacked, Hush was quoted, 'The objections resolve themselves into the question whether *Honi Soit* is to be permitted to publish material that may arouse controversy—that is, whether it is to give principal attention to the truth or to people's feelings. We cannot have controversy without paining people who have prejudices. I am sure that the anti-liberal forces will not meet with success' (Anonymous 1945; Hector 2019).

Postgraduate research at university of Sydney

Academic staff numbers at Sydney had been depleted during World War 2, during which much of the effort of those remaining had been diverted into war-related work, especially by the organic chemists producing pharmaceutical compounds. But some research continued—in his AAS interview, Hush mentioned a staff member who had 'just come back from working with Linus Pauling in California, which was a big thing'. This was David Mellor (1903–1980) (Baker 2021). Entering his Honours year in 1945, Hush was offered a range of research projects, from which he chose to work on semiquinones with organic chemist G. K. Hughes and David Mellor. The work concerned the products of one-electron oxidation of *p*-phenylenediamines and their polymerisation, for which chemical structures had been proposed by Michaelis and Granick (Michaelis and Granick 1943). These proposals, however, were queried by Hughes and Hush (Hughes and Hush 1947), who prepared new salts of these radical cations, and measured their magnetic moments and their catalytic reduction by hydrogen. It was the view of Michaelis and Granick that at least one N-H group in the diamine was necessary for the oxidation to occur, but further work by Hush showed that a diamagnetic semiquinone could be formed by oxidation of tetramethylbenzidine that had no such hydrogens (Hughes and others 1947).

In his AAS interview, Hush said that this work 'embodied something which has been occupying me ever since—the ways in which nuclear and electronic motions become mixed up with each other'. Supported by a junior lectureship, he published results of research on a range of physical chemistry topics (see Supplementary Material) that in other circumstances might have earned him a PhD, but were sufficient for the award of an MSc degree. The first Australian PhDs were awarded by the University of Melbourne in 1946, but it was 1951 before the degree was awarded at the University of Sydney (Rae 1999).

Manchester

Seeking financial support to undertake postgraduate study in UK, Hush applied to both University College London (UC) and to the University of Manchester for ICI Fellowships that had been offered by Imperial Chemical Industries since 1944 (Rae 1994). He would have been aware that Alan Maccoll, a year ahead of him at Sydney, had been awarded an ICI Fellowship to undertake research for his PhD under Christopher Ingold (1893–1970) at UC, and that David Craig had completed his PhD there and remained on the staff as a research fellow. At Manchester, his aim was to work with theoretical chemist M. G. Evans (Melville 1953). Neither application was successful, but Evans wrote to him[2]

[2]International Telegram, MG Evans to NS Hush, 22 May 1949. Letter, MG Evans to NS Hush, 4 June 1949, correspondence held by JR Reimers.

saying that, 'there is so much in common on your work on heats of solution of ions and oxidation reduction studies with my own', and offered a three-year appointment as an Assistant Lecturer that would 'provide ample opportunity for research'. This was an emergency appointment, not requiring interview and within the power of the professor to make. Hush accepted promptly and later explained to Max Bennett, Professor of Neurology in the University of Sydney medical school, that he chose Manchester rather than Oxford or Cambridge, where Australian scientists were wont to go for postgraduate studies, because of its strength in those fields, having been home to 'greats' like Ernest Rutherford, Ludwig Wittgenstein, and Michael Polanyi (Bennett and Reimers 2019). With his fiancée, Thea (daughter of Leslie and Mary Warman), travelling in R.M.S. *Ormonde* Hush arrived late in 1949 to take up his appointment in the new year. He was co-author with Evans on a major review of radicals and ions involved in reactions of hydrogen peroxide, and he published two papers on electrochemically-generated free radicals. His molecular quantum calculations of the properties of aromatic hydrocarbons began at Manchester were only completed and published after he had moved to Bristol (see below). In contrast to the lingering effect of post-war restrictions and the notoriously poor weather, Hush found the scientific environment at Manchester very stimulating. Among his colleagues were Michael Kasha, Christopher Longuet-Higgins, and John Polanyi (and in another department, his philosopher father, Michael Polanyi), all of whom went on to prominence in the field of theoretical chemistry.

Alan Turing, of code-breaking fame, was a member of the department of mathematics at Manchester, where he was working on a theory of biological morphogenesis—'how living things get their shape and their function', as Hush put it—that was based on coupled diffusion-reaction mechanisms. Hush was also studying these in the context of heterogeneous electron transfer, and the two engaged over lunch in discussions about the basic theory. The publication of Turing's work (Turing 1952) did not attract much notice when it was published in 1952, but is now highly regarded as a cornerstone of this important aspect of biological growth.

At Manchester, Hush (Fig. 2) adapted the chemical reaction-rate theories that had been developed there by Polanyi using reactive potential-energy surfaces, to consider instead reactions involving electron transfer that had only small associated changes in structure (Evans and Hush 1952). These, he reasoned, could be described using much simpler harmonic (parabolic) surfaces that were coupled together.

Boristol

With the death of Meredith Evans in 1952, those who had been working with him moved to other institutions. Hush's assistant lectureship was extended by a year, but by 1954,

Fig. 2. Hush at Manchester 1953 (Hush family).

he had taken up a position at the University of Bristol where he worked with Professor M. H. L. Pryce (1913–2003) (Elliott and Sanders 2005), the head of department who had come from the Chair of Theoretical Physics at Oxford University and was a specialist in crystal field theory that Hush said, 'was revolutionising our understanding of the electronic structure of transition metal ions'. Within this conceptual field, Hush undertook research on electron transfer processes about which he was able to make quantitative predictions. As well as those involving electrochemical processes, Hush studied optical transitions that involved transfer of an electron from a donor to an acceptor, both of which possess more than one accessible oxidation state ('intervalence transfer'). The process was 'homonuclear' when ions of the same metal were involved, or 'heteronuclear' as in a normal oxidation-reduction pair. An example of the former was the complex iron cyanide known as Prussian blue, and of the less common heteronuclear type, the intensely coloured Pd^{II}–Pt^{IV} compounds (Allen and Hush 1961; Hush 1961*b*).

In 1959 Hush submitted twenty-one published and submitted papers on 'Electronic structure and stability of inorganic and organic ions and molecules, and electrochemistry' to the University of Manchester in support of his application for the award of a Doctor of Science degree. The degree was awarded, following the university's receipt of strong support by their referees, who noted that he had 'seized promptly upon important ideas and tackled topical if difficult problems' and, noting an unusual characteristic of Hush's research, that 'the problems have been well chosen with a view to comparison with experiment, and the relevant experimental data have been critically examined' and that 'in two of the fields of investigation there is an admirable fusion of theoretical and experimental approaches', the latter requiring 'a fair degree of skill', and thus 'achieved an authoritative standing in both' by 'the drawing together of related experimental information into a coherent and reasonable satisfactory scheme'.

Hush's major work was presented at the influential Fourth Moscow Conference of Electrochemistry 1956, from which the proceedings were translated into English in 1961 (Hush 1961*a*). This work was also submitted for mainstream publication, with publication delays resulting in a 1958 publication (Hush 1958). Its core element was that electron transfer was perceived as proceeding slowly as the atoms moved adiabatically, in accordance with the basic principles of quantum mechanics, and was subject to calculation by *ab initio* means. The continuous electron transfer aspect was a measurable effect that controlled both spectroscopy and electrochemical reactions. During the publication delay, a critical paper on electron transfer was published by Marcus in 1956 (Marcus 1956) based upon his (unphysical) non-adiabatic theory of electron transfer in which the electrons were perceived to transfer instantaneously, which nevertheless delivered a major result. Then in 1959–60, Levich and Dogonadze independently developed their own adiabatic electron-transfer theory, which is formally equivalent to Hush's theory, and applied it to determine the rates of very slow processes in the non-adiabatic limit (Levich and Dogonadze 1959, 1960). The combined works of Hush, Marcus, and Levich and Dogonadze define the basics of electron-transfer theory as we know it today, with the Russian authors also acknowledging the fundamental work of Kubo and Toyozawa (1955).

In 1962 when Hush had been a visiting scientist at the Brookhaven National Laboratory in the United States, he paid particular attention to a case where the metal ions shared a bridging ligand in their inner shells, a situation that he felt was probably common in biochemical processes involving electron transfer across large organic molecules (Hush 1963).[3] The paper was submitted to *Inorganic Chemistry*, but was rejected on the advice of a reviewer who subsequently identified himself as Rudolph Marcus. It would appear that the paper was never published formally, yet its content indicates the building blocks for Hush's subsequent understanding of intervalence spectroscopy, and then the properties of the Creutz-Taube ion that is described later in this biographical memoir.

Hush was later to extend his ideas that electron-transfer always happened continuously, to point out that, even in the initial and final chemical states, the electron was always slightly transferred. This would have consequences for spectroscopy, as light could manipulate the partly-transferred state of the electron. This led (Hush 1967) to Hush's explanation of Robin's 1962 interpretation of the distinctive, but unexpected colour of Prussian blue, the world's first synthetic dye. Robin assigned the transition to intervalence charge transfer of an electron from Fe^{II} ions to Fe^{III} ions located a long distance away inside the crystal, and Hush's theory explained how this was possible. These works, and the review in the same year by Robin and Day (1968), initiated the modern research field of mixed-valence chemistry.

A definitive example of Hush's ideas—the Creutz-Taube complex—was prepared two years later year by Carol Creutz working in the laboratory of Professor Henry Taube at Stanford University. It was a symmetrical binuclear ruthenium complex in which the metal ions in valence states II and III respectively were connected by a pyrazine ring, $(H_3N)_5Ru\text{-}NC_4H_4N\text{-}Ru(NH_3)_5{}^{5+}$ (Creutz and Taube 1969). Absorption in the near infrared, λ_{max} 1570 nm, was ascribed to the transition (using the authors' notation) [2,3] → [3,2]*. Half-oxidation of the [2,2] complex had been performed in Taube's laboratory, but since no colour change was observed, the matter had not been further pursued (Ford and others 1968). Taube, in his Nobel Prize lecture (Taube 1983), observed of Creutz's work that 'the review papers by Hush (Hush 1967) and Robin and Day (Robin and Day 1968)—had appeared, and taking their content to heart, we felt certain that an intervalence band must exist, which Carol Creutz then located in the near infrared region' (Taube 1983). Taube also wrote privately[4] to Hush, thanking him for his congratulations on the award of the Nobel Prize, and taking 'this opportunity to acknowledge my special debt to you. Particularly in the work on mixed valence molecules, your insight has guided my footsteps'. Considering the properties of the Creutz-Taube ion, it soon became clear that the electron resided half on each ion, however, providing the perfect example of Hush's concept that electron-transfer processes always happen continuously rather than instantaneously; debate about the details of this continues to this day.

Looking back on the way the field had developed, Hush (1982) reflected on the increase in information, derived from experiments, about the rates of electron-transfer and the fact that this had been critical in helping theoreticians to assess the value of different approaches. He was aware that the story was not yet complete, and outlined some of the outstanding theoretical issue awaiting resolution.

Sydney

In 1969 the University of Sydney took advantage of some chairs being vacant to loosen the department structure by 'seeking appointees on the grounds of merit above their linkage to traditional subdivisions of chemistry' (Branagan and Holland 1985). The first to be advertised was a chair of theoretical, macromolecular or analytical chemistry, and an Advisory Board was appointed to consider applications for

[3]The paper 'The Function of Bridging Groups in Electron-Transfer Reactions' is accessible at the UNT Digital Library, https://gigital.library.unt.edu/ark:/67531/metadc1250504/?q=hush, viewed July 2025.

[4]H Taube to NS Hush, 27 October 1983, correspondence held by JR Reimers.

two chairs. In its report to the Professorial Committee, the committee recommended the appointment of Sydney graduate Noel Hush to a chair of Theoretical Chemistry. This advice was accepted by the Senate at its July 1970 meeting and following his acceptance Hush's appointment was confirmed in July 1971. Hush had also applied for the inorganic chair, which went to the internal candidate, Hans Freeman in March 1971. Ernest Ritchie (1917–76) continued as professor of organic chemistry, while Walter Moore became professor of physical chemistry in 1973.

In his interview with the Academy of Science, Hush commented that he was ready to leave Bristol where he had been 'embedded' for fifteen years, and the obvious place to go was the United States (US), but 'for family reasons, that was out'. Hush had been a frequent visitor to the US, but on only one occasion did his family travel with him, when he held a visiting position at Florida State University in Tallahassee in the American autumn of 1965.

He had an opportunity at Sydney to start a new department of theoretical chemistry that would be the only one in Australia. It was an initiative, Hush said, of the Chancellor, Bruce (later, Sir Bruce) Williams, a former staff member of the University of Manchester. Negotiations over the conditions of his appointment were conducted with Williams by telegram because of an extended mail strike in Britain at the time, and the warm relationship between the two that developed was continued when Hush arrived in Sydney (Hush 2010). Once there, he was soon able to appoint the likes of Robert Gilbert, Sture Nordholm, George Bacskay, and Pieter Schipper, and with them, to implement a vigorous undergraduate teaching course and a productive research programme that attracted talented students, many of whom went on to highly successful careers in theoretical or experimental research.

Hush and Russian Jewry

In April 1972, not long after he took up his chair at the University of Sydney, Hush received an open letter from two Russian Jewish professors, Alexander Voronel (Anisimov and others 2025) and Benjamin Levich (1917–87) (Acrivos 1992), who urged their colleagues in the west to protest the practice of detaining specialists in the USSR. Hush, a non-Jew, was particularly concerned with the fate of Benjamin (Veniamin) Levich, a theoretical electrochemist whom he had met at the 1956 Electrochemistry Conference in Moscow and maintained contact with over their mutual research interests. Levich's application to leave the USSR and accept an offer of a chair at Tel Aviv University had been denied: he was stripped of his academic position and his 'Academician' status, and denied communication with national and most international peers. His son, Eugene (Yevgey), an engineer, had also been refused the right to apply for an emigration permit. Responding to the letter, Hush sought to enlist the heads of chemistry and physics departments at Australian universities, and he also telephoned Levich to express his support (Anonymous 1972*a*).

The dilemma for Russians—'refuseniks', as they came to be known, many of them Jewish and wishing to resettle in Israel—was of long standing (Lipski and Rutland 2015), and it was worsened in August 1972 when the USSR introduced head taxes with amounts, often many thousands of pounds, scaled to reflect the professional and technical qualifications they had achieved in the Soviet Union. Governments, professional societies, and scholars in the western world protested this imposition. In Australia, public attention was drawn to it by an editorial in the *Sydney Morning Herald* (Anonymous 1972*b*), and this was quickly followed by a letter to the editor of the newspaper by three University of Sydney academics—Upendra Baxi, a senior lecturer in Law; Noel Sydney Hush, professor of theoretical chemistry; and Julius Stone, professor of international law and jurisprudence (Baxi and others 1972) expressing their wish to appeal to the Soviet government to withdraw the tax, and inviting colleagues in Australian tertiary institutions who wished to be associated with this to contact them. The cases of Benjamin Levich and his son were cited, the latter described as 'disappeared and presumed kidnapped'. Hush was identified in two items in the *Australian Jewish Times* (Anonymous 1972*c*, 1972*d*) as the leader of the Sydney group.

Hush was not mentioned in the report of a letter of protest, initiated by the Australian Association for Cultural Freedom and signed by 71 Australians (including Julius Stone) that was mailed to Soviet leaders in October (Anonymous 1972*e*), but he headed the list of nearly 300 Australian academics who signed an appeal that was cabled later in the month to Soviet President Nikolai Podgorny (Anonymous 1972*f*). A petition was also sent by Australian parliamentarians; another by academics convened by Flinders University professor of social psychology, Leon Mann; and two hundred people demonstrated outside the Australian parliament in September. Lipsky and Rutland commented that Levich 'became a symbolic figure in the protests' (Lipski and Rutland 2015, p. 112).

Hush was again on the telephone to Levich a year later (Gottshall 1973), when he was joined by the President of Tel Aviv University, Professor Yuval Ne'eman (1925–2006), a theoretical physicist who was in Australia to attend the General Assembly of the International Astronomical Union in August, and to visit researchers at the University of Melbourne. Levich told them that he remained interested in science, but his former colleagues had shunned him, leaving him alone in the room to read scientific journals. He and his wife, Tanya, who was also in the call, expressed thanks for the encouragement and support. The Levich's sons with their families were allowed to leave in 1975, but the parents were detained—on the grounds that Levich was in possession of state secrets—until 1978, when they moved not to Israel, but to New York where Benjamin took up a university position.

Research at the University of Sydney

The volume of research published by Hush and his co-workers over four decades makes it impossible to comment on many individual papers; his major interest in electron transfer is obvious from the titles of his published works (Supplementary Material). The names of his co-authors reveal the extent of his collaborations with experimentalists and other theoreticians, but it is important to note here the contributions made by two major associates, George Bacskay and Jeffrey Reimers.

Bacskay, a Melbourne graduate who completed his PhD with J. W. Linnett at Cambridge in 1971, joined Hush in 1972 as a post-doctoral fellow with a brief to supplant the semi-empirical methods of computation used by Hush with the more advanced *ab initio* methods he had developed at Cambridge. At the end of 1972 he accepted a permanent position as 'Programmer' in the department, with the understanding that 'I would continue calculations, my *ab initio* work, give a course of tutorials throughout the year on Quantum Mechanics and Quantum Chemistry, help with the supervision of graduate students in that area, generally provide computational assistance to staff and students in the department and last (but not least) give a lecture course on Fortran Programming to our third year Chemistry undergraduates'. When Hush retired, Bacskay's position was re-classified as Research Fellow and a few years later, he joined the teaching staff in the School of Chemistry as Senior Lecturer, teaching at all levels but predominantly in the area of Spectroscopy and Quantum Chemistry. He retired as a Reader in 2005, by which time he had published 57 papers with Hush.

Reimers (PhD ANU 1983) joined the Theoretical Chemistry Department in 1985, having studied spectroscopy with Ross and Craig, and thermodynamics and quantum spectroscopic simulations of liquid water with Bob Watts, and following postdoctoral experience with theoretical chemists in the United States. From 1989 until the death of Hush thirty years later, they co-authored 130 papers. Reimers was elected to fellowship of the Australian Academy of Science in 2010, and was recipient of its David Craig Medal in 2016. In the text of his award lecture (Reimers 2016), he linked aspects of Hush's research to that of Craig, whom he described as a pioneer in theoretical chemistry, who had a profound impact on the development of the science in Australia.

To demonstrate the breadth of topics addressed by the theoretical chemists and their experimental collaborators, we have selected aspects of the research conducted in the Sydney years that highlight their results and give insight into the way they worked.

Molecular electronics

A centrepiece of Hush's theory of electron transfer was that the properties it described were all subject to *ab initio* computation based upon the fundamental principles of quantum mechanics. Backsay turned this dream into reality. His work with Hush focused on the interaction of molecules with electric fields, either static electric fields or else the electric field of light. In Hush's first publication at Sydney University, they developed the methods needed to make the first *ab initio* calculation of molecular responses to applied electric fields (Bacskay and Hush 1974). A subsequent germinal paper in this area, which was also one of the first papers to include Reimers, showed how applied electric fields could be used to induce intramolecular chemical reactions (Hush and others 1990). This work, the pioneering work of Aviram and Ratner (1974), and the invention of scanning-tunnelling microscopy (STM) in the 1980s, led to the new burgeoning field of molecular electronics. Hush was a recognised leader in the field internationally and nationally, driving a Commonwealth Department of Science sector review of the new technology in 1988. The dream was that single molecules could replace silicon in electronic circuits.

Paralleling this, molecular electronics was also making headway in chemical and biochemical research, pioneered by Steven Boxer, with whom Hush established a life-long friendship. Boxer had invented a new way of implementing Stark spectroscopy, allowing for unprecedented electric field strengths to be applied. Hush and Reimers pioneered the interpretation of these experiments (Reimers and Hush 1991). Later, Boxer would become the first person to give the endowed Hush Lecture at Sydney University, and also the plenary speaker at the RACI 2024 meeting in honour of Professor Hush (Supplementary Material).

Molecular electronics remains a significant research field in Australia. This was highlighted by a symposium at the 2022 RACI National Convention and subsequent review article by Reimers and Low (2023).

Photosynthesis models: collaboration with Michael Paddon-Row and Jan Verhoeven

Michael Paddon-Row at the University of New South Wales, starting in the 1980s, had prepared a series of rigid molecular frameworks that enabled him to study one-electron orbital interactions through space and through carbon-carbon single bonds (Paddon-Row 1982). Paddon-Row was interested in working with experimentalists to explore the photo-excitation and decay processes taking place in these systems, such as Ken Ghiggino at the University of Melbourne (Lawson and others 1993), but also with theoreticians with whom he could advance the understanding of them. His first link of this type was with P. E. (Eddie) Schipper, a member of the Department of Theoretical Chemistry at Sydney, and they published the results of their investigations in 1982 (Schipper and Paddon-Row 1982). It was through Schipper that Hush met Paddon-Row, and realised that he and Jan Verhoeven had produced results for which he, Hush, had developed relevant theory. This led to more extensive collaboration between the three of them and their respective colleagues (Hush and others 1985; Oevering and others 1988).

The centrepiece of this work was the ability of the Paddon-Row molecules to absorb light locally at one end, producing excited electrons and holes, with then either the electron or hole transferring by intramolecular electron transfer to the other end. This 'charge-separated state' could be thought of as being like a battery, storing holes and electrons in different locations. Analogous processes are used by chlorophyll and related molecules to capture solar energy and convert it into chemical energy during photosynthesis. The key aspects of how this happened were unknown at the time, and the work of Paddon-Row, Verhoven, and Hush demonstrated the basic required elements (Hush and others 1985; Oevering and others 1988). The observed rates for the electron transfer did not fit that expected purely from Hush's theory of electron transfer, leading to his collaboration with Reimers, who was brought in to use his spectroscopic background from his Ross and Craig years to explain the discrepancy (Reimers and Hush 1990).

Photosynthesis

By the 1990s, Hush's adiabatic electron-transfer theory, the work with Bacskay in *ab initio* calculations of the effects of electric fields, and the revealing experiments of Paddon-Row and Oevering had made the understanding of natural photosynthesis a practical objective. A critical paper was published by Breton in 1992 (Breton and others 1992) showing astonishing spectra of the reaction centre in purple bacteria containing a broad absorption sitting amidst the usual infrared absorption spectrum. Reimers describes Hush as 'coming into his office one day, putting the spectrum on his desk, and asking, as one would do to an undergraduate student, "what is it"'. Reimers replied 'it's the intervalence charge-transfer spectrum', wondering why such an obvious question pertaining to Hush's famous description of Prussian blue had been asked. 'Well then prove it!', demanded Hush. The trouble was that the intervalence spectrum had already been assigned to another transition at much higher energy. Also, the bacterial proposal violated a minimum-energy requirement set by previous exhaustive experiments. These involved application of site-directed mutagenesis to modify the electric field across the reaction centre and then recording the electrochemical potential of the centre and its electron-spin resonance spectra. The result was identified of how the charge on the associated bacteriochlorophyll dimer cation was distributed, leading to the setting of a lower bound for the coupling and hence the intervalence transition energy. Solving these issues took a decade of research, often involving protein simulations and the effects of its internal electric fields. The result was a model that explained all of the observed features of the reaction centre (Reimers and Hush 2004). Of note, this was a full quantum model that involved fractional electron occupancies, a critical element of Hush's 1958 theory, with no description of the system in terms of 'molecules' and 'ions' being tenable. This is one of the few occasions in which a non-trivial quantum effect has been shown to be critical to biological function.

A controversial prediction of the model for bacterial photosynthesis was that the observed spectra would change dramatically as a function of an applied electric field. Steven Boxer later verified these predictions (Kanchanawong and others 2006), establishing a key result in quantum bioscience.

New devices: porphyrins with Maxwell Crossley

In 1991 Hush and Reimers began a collaboration with their University of Sydney colleague, Maxwell Crossley—a master of porphyrin synthesis—that was to extend over 25 years and yield fifteen publications in molecular electronics arising from the combined efforts of their research groups. The chlorophyll and bacteriochlorophyll molecules that control natural photosynthesis are modified porphyrins, so this type of research was envisaged as leading to new generations of practical devices. Concluding the first of their joint papers (Binstead and others 1991), the authors wrote, 'A brief comment on the relevance of these results to the design of proposed molecular electronic logic or memory devices, in which there is a current surge of interest, in which porphyrins or polyporphyrin systems could play a role in electron/hole or energy transmission, is in order…. Where porphyrins are involved in the design of such devices, it should be possible to incorporate and predict sensitive tuning by appropriate pyrrolic β-substitution employing the principles outlined above'. Their exploration of the possibilities for electron transport offered by porphyrins, published in 1994 (Lü and others 1994), revealed that there was weak inter-unit coupling between conjoined porphyrin rings that was readily tunable. 'Compared to other possible molecular wires', the authors concluded, 'these have the striking advantage of spanning large distances', citing the 56 Å span in one of their compounds. 'Hence, a little coupling goes a long way, and these molecules are expected to possess many practical advantages over alternative systems.' Many difficulties lay in the way of operationalising these 'molecular wires', one of them being the appearance of polymorphs in the self-assembly of monolayers of some candidate porphyrins, as described in the final publication of this collaborative series (Reimers and others 2016*a*). Polymorphs that could 'crystallize' in an ordered and predictable way when the alkyl chains in meso-tetraalkylporphyrins contained fifteen or more carbons.

The work led to an Australian Research Council Linkage Grant with the Intel company, seeking to make new molecular memories. Reimers comments that, 'most, but not all, research milestones were met, inhibiting the next steps but also making publication or patenting unsuitable as this would encourage commercial competitors'. This dilemma faces many scientists today as basic science advances are translated into commercial products. The work involved setting up a scanning tunnelling microscope (STM) laboratory at the University of Sydney. Published work included the development of basic understanding of the way that functionalised monolayers form on surfaces (Reimers and others 2015)

Advanced scanning-tunnelling microscopy: collaborations with Jens Ulstrup

Jens Ulstrup from Denmark had made many significant contributions to molecular electronics, and was strongly connected to the Russian tradition of adiabatic electron-transfer theory, dating back to the pioneering works of Levich and Dogonadze. Ulstrup recalled that his first personal contact with Professor Hush was in Padua, Italy in 1992, at a Molecular Electronics conference, an area to which Hush and Reimers were already strong contributors. He immediately got on very well with Hush, and their contact was strengthened at a later conference, *Electron and Ion Transfer in Condensed Media – Theoretical Physics for Reaction Kinetics* at the International Centre for Theoretical Physics (ICTP) in Trieste, 1996. Just before the meeting, Ulstrup discovered that his fellow organisers had allocated to him the daunting task of starting the meeting with a story on 'The History of Chemical Charge Transfer'. To his great relief, when the conference proceedings were to be published in full, Hush consented to help with the completion of this challenging chapter (Hush and Ulstrup 1997).

The next year (1997), Hush and Ulstrup both attended the *Fast Reactions in Solution* meeting in Copenhagen, where their friendship developed. This led to Ulstrup spending his sabbatical at the University of Sydney in 2003, at the time that Hush, Reimers, and Crossley were planning their STM facility.

Ulstrup, with colleague Jingdong Zhang, had built the state-of-the-art facility for studying electrochemistry at atomically planar single-crystal electrode surfaces, with in particular scanning tunnelling microscopy and spectroscopy under full electrochemical potential control (*in situ* or *in operando* STM and STS). This delivered some of the highest resolution spectra ever produced for *in situ* STM images, and both *in situ* current/overpotential and current/bias STS correlations at the level of the single molecule. The target molecules were small: functionalised alkanethiols in particular, but also complex redox molecules, transition metal complexes and the metalloproteins cytochromes, blue copper proteins and iron-sulfur proteins. Ulstrup recalled:[5]

> We had also developed phenomenological theory for *in situ* STS of redox molecules. Conceptual and theoretical challenges are that what is registered are tunnelling *currents* rather than molecular *structures*. Even the prettiest STM images are therefore at risk of reducing to mere blops unless supported by heavy theoretical and computational frames that convert tunnelling currents to molecular structures. Professors Hush and Reimers, with their associates (A Bilič, RH Ouyang, Y Wang) took interest in such much more detailed *in situ* STM image interpretation, and in a series of heroic efforts they could map out the images in novel amazing detail also triggering new experimental efforts.

The collaboration between Hush, Reimers, and Ulstrup led to fundamental understanding as to how sulfur-bound molecules self-assemble on gold surfaces and nanoparticles, stressing its prominent van der Waals character (Reimers and others 2016*b*, 2017). How materials self assemble on surfaces is critical to the understanding of how they conduct electricity in molecular electronics, and how applied electric fields control their isomerism.

The Penrose-Hameroff theory of consciousness and student McKemmish

Mathematician Roger Penrose, in *The Emporer's New Mind* (Penrose 1989), had considered the idea that consciousness might be a quantum phenomenon. Beginning with a discussion of the conventional model of neurotransmission within axons by polarisation of electrolyte concentrations, and between their synapses by chemical flow, he moved in sections entitled 'is there a role for quantum mechanics, in brain activity' and 'quantum computers', to speculate that single-quantum-sensitive neurons might be playing an important role deep inside the brain, but concluded that so far this idea did not look very promising. He elaborated on the concept in his *Shadows of the Mind* (Penrose 1994), and it was taken up by anaesthetist Stuart Hameroff, who worked on it with Penrose (Penrose and Hameroff 1995). Together they felt that late twentieth century views of consciousness, in which neural activity in the brain was held to be a function of chemical interactions between neurones, set unrealistic limits on processing capacity, and they proposed a new model of cognitive function in which the driving force was quantum computation in microtubule assemblies within neurons. Their theory, known as Orchestrated Objective Reduction (Orch OR), involved pairs of microtubules in two conformational states, resonance coupled so as to constitute a qubit as a result of superposition of the local vibronic wave functions. There was extensive debate about this idea, which attracted some support from the scientific community, but also much criticism. According to their postulates, consciousness arose as a complex quantum effect involving a combination of quantum biochemical dynamics and quantum gravity. Aspects of their work showed strong overlap with the quantum theory for the operation of

[5]Ulstrop, private communication July 2025.

bacterial photosynthesis developed by Hush and Reimers, making this a feasible area for their research.

Combining with the biochemical simulator Alan Mark, the quantum physicist Ross McKenzie from the University of Queensland, and first-year undergraduate student Laura McKemmish, they set out in 2009 to verify their proposal using quantum biochemical simulations. They showed that the Penrose-Hammeroff model was untenable because, (1) the biochemical model which underpinned it was incorrect (McKemmish and others 2009), and (2) its evocation of quantum coherence following the production of a Fröhlich condensate was not feasible (Reimers and others 2009). Fröhlich, a great mid-twentieth century innovator closely associated with the development of superconductivity and Bose-Einstein condensation, had proposed that a system with energy constantly flowing through it could lead to a highly ordered non-equilibrium state, with nearly all of its vibrational energy concentrated in the motion of lowest frequency. This condensate Fröhlich had assumed to be quantum coherent, providing a centrepiece for the Penrose-Hameroff proposal. Hush and his collaborators verified Fröhlich's assertion that a condensate would form, but showed that it would be extremely unlikely to be quantum coherent, and, 'As a result', they wrote, 'while the Penrose-Hameroff proposal holds the fascinating possibility of quantum mechanical effects playing a central role in cognitive function … it does not hold … and we hope that with this work we can finally put to rest this intriguing but fundamentally flawed model'. Their work was quoted in the USA TV sitcom 'The Big Bang Theory', Season 3, Episode 11, in 2009.

Penrose and Hameroff revised and defended their work in a lengthy review (40 pages and 176 references) (Hameroff and Penrose 2014*a*) in an issue of the journal *Physics of Life Reviews*, which also included several commentaries on it. One of these was from the Hush team (Reimers and others 2014), who examined the arguments in the Penrose-Hameroff review, and concluded that it 'is thus neither self-consistent nor scientifically coherent and violates the basic tenants of good scientific practice'. Facing with this stinging comment, Hameroff and Penrose provided a line-by-line response (Hameroff and Penrose 2014*b*). The propensity of these authors to invoke and engage in robust debate had been evident for many years. For example, Hameroff had made a similar rebuttal of the provocative views about the Penrose-Hameroff proposals expressed by Patricia Smith Churchland (Churchland 1998), who wrote that 'Penrose and Hameroff are offering a make-believe pig in a fantasy poke' because 'pixie dust in the synapses is about as explanatorily powerful as quantum coherence in the microtubules'. Hameroff rebutted her logic point by point, and ascribed her anti-quantum view to 'reaction to her biology teacher—an avowed vitalist!' (Hameroff 1998).

As the debate descended from scientific argument to personal invective, the Hush group decided to cease work in this area. Before leaving this story, however, we should link it with something that Reimers said about Hush, that 'a central focus of his time at Sydney University was on student teaching and early career researcher mentoring' (Reimers 2019). Hush's encouragement of Laura McKemmish, first author on a 2009 paper, is a case in point. She began her association with the group as a first-year undergraduate undertaking a student project with them, and continuing the connection through her baccalaureate studies, since which she has pursued a career in theoretical chemistry with her own research group at the University of New South Wales.

Other notable students: John Dyke, Peter Taylor, Jill Gready, Jun Zeng, and Gemma Solomon

Very many students were influenced by Hush over his long career, either as their supervisor, mentor, friend, or acquaintance, too many to list. We consider five who went on to do significant things and remained in close contact.

John Dyke was a student at Bristol, going on to be a spectroscopist at Southampton. He was a strong advocate for Chemistry, winning a Royal Society of Chemistry advocacy prize.

Peter Taylor and Jill Gready were two of the first students at the Department of Theoretical Chemistry at Sydney, working also with George Bacskay. Taylor developed new methods in computational chemistry (Taylor and others 1976), and went on to develop supercomputer centres in USA, Australia, and China. Gready was a pioneer of the development of electric-field methods in computational chemistry (Gready and others 1977), and went on to become a professor in the John Curtin School of Medical Research at the Australian National University, pioneering medically related research in computational chemistry.

Jun Zeng and Gemma Solomon were students some 20 and 35 years later, working also with Jeffrey Reimers. Zeng studied how the electric fields from condensed-phase environemnts affected molecular properties (Zeng and others 1993). He went on to be one of the six authors of the patent for the drug 'momelotinib', one of the most significant Australian pharmaceutical developments, that led to the Prime Minister's Prize in 2024 for the team leader, Professor Andrew Wilks. Gemma Solomon developed a theory to explain how vibrational spectra of alkanedithiols adsorbed on gold can be measured using single-molecule conductivity experiments (Solomon and others 2006), and went on to be a leader at Copenhagen University in both molecular electronics and nanotechnology.

Relocation to the School of Biochemistry

Reaching the then-customary age of retirement (sixty five years) in 1989, and wishing still to continue research, Hush encountered the university policy that senior professors and heads of department at that point were obliged to relocate so as to lessen any opportunities they had to interfere in the running of their old department. Thus, Noel Hush moved to an office in the School of Biochemistry, where he made new friends and found new collaborators. Not all of the collaborations were about science. In 2016 Building G08, constructed for the biochemists in 1970–3 in the 'brutalist' style, but in 2010 renamed Molecular Bioscience, was slated for demolition. While many did not admire its heavy, concrete style (Fig. 3), others thought that such a fine example of the style deserved retention and refurbishment. One of those was Noel Hush, who suggested to his biochemical colleagues Professors Richard Christopherson and Philip Kuchel that they seek heritage status for it. In this cause Hush wrote to his friend Clive Lucas, a prominent Sydney restoration architect who was at that time President of the National Trust, and met with him to press their view. Formal submission by Kuchel led to listing of the building by the National Trust of Australia (New South Wales). British architectural historian Christopher Beanland had included the building in his book on brutalist architecture around the world, noting that the

Fig. 3. Two views of the Molecular Bioscience building at the University of Sydney (Philip Kuchel).

style was well represented in Sydney, with the School of Molecular Biosciences & Biochemistry 'the pick of the bunch' (Beanland 2016).

Australian Academy of Science

Hush served on the Academy's sectional committee for chemistry 1978–89, being chairman 1981–2; on the science policy working group 1987–1997; and during 2006 on the selection committees for the Lèvre and Craig medals. He was honoured on two occasions, first, in 1994 by the award of the Matthew Flinders medal for research in physical sciences, and in 2000 he was the inaugural David Craig medallist, awarded for outstanding contributions to research in chemistry.

Royal Australian Chemical Institute (RACI)

Soon after returning to Australia, Hush joined the Royal Australian Chemical Institute (RACI) and was a regular contributor to the research conferences of its Physical Chemistry Division (Fig. 4).

Honours and awards

A full list is provided in Supplementary Material, but the most significant of Hush's honours were his election to Fellowship of the Australian Academy of Science in 1977, the Royal Society of London in 1988, and in 1993, his appointment as an Officer of the Order of Australia (AO) for 'For service to science in the field of theoretical chemistry'; and his election as an Honorary Foreign member of the American Academy of Arts and Sciences.

Two major awards came late in Hush's career. The first was in 2007 when the Welch Award in Chemistry was made jointly to Noel Hush and William H. Miller of the University of California, Berkeley, for their lifetime achievements in theoretical chemistry. The recipients shared the $US300,000 prize from the Robert A. Welch Foundation in Houston, Texas. In his award paper (Hush 2008), Hush cited the results of his own research published between 1951 and 2003, and provided a thorough review of the development of the field, structured around four revolutions that contributed to his understanding of the basic nature of electron or hole transfer processes—molecular orbital formalism replacing the Pauling valence-bond 'resonance' description of electronic structure; electron paramagnetic resonance spectroscopy shows spin and charge delocalisation to ligands; transition state (absolute reaction rate) theory; crystal field theory and the renaissance of inorganic theory—and a subsequent four that brought scientists closer to an understanding of these processes—ligand-bridged electron and hole transfer; introduction of ultrafast spectroscopic techniques; computers; and nanotechnology - venturing into Feynman's 'room at the bottom': molecular electronics.

In 2014 Hush received the Ahmed Zewail Prize for Molecular Science. This biennial award is sponsored by Elsevier in collaboration with the international journal *Chemical Physics Letters*, honouring their Honorary Advisory Editor, Professor Zewail, who received the 1999

Fig. 4. Noel Hush and Gen Ghiggino (University of Melbourne) at the RACI Physical Chemistry conference in Yeppoon, Queensland, in 2007 (Angela Ghiggino).

Nobel Prize in Chemistry for his investigations of fundamental chemical reactions on the femtosecond time scale.

Celebrations

The Hush Fellowship Fund was established by the School of Chemistry in 2005 for the purpose of holding annual lectures by noted international scientists in the area of Professor Hush's research interests, to commemorate his great scientific achievements. Hush Lectures were delivered by Abraham Nitzan, Tel Aviv University (2009); David Clary, University of Oxford (2014); Steven Boxer, Stanford University (2015); and Benjamin J. Schwartz, University of California Los Angeles (2024).

A symposium to celebrate his eightieth birthday was held at Sydney University in 2005, and the presented talks, edited by Reimers, Ulstrup, Solomon, and Hush's friend and key electron-transfer experimentalist Thomas Meyer, were published the following year in two special issues of *Chemical Physics* under the heading, 'The Molecules and Methods of Chemical, Biochemical and Nanoscale Electron Transfer' (Reimers and others 2006*a*, 2006*b*). People contributed from Australia, Asia, Europe, and the US. A noteworthy attendee was Alexander Kuznetsov, who brought home to the audience the close connection between the Hush and the Levich-Dogonadze adiabatic theories of electron transfer.

There were three symposia held in his honour after his death in 2019, pointing to his enduring legacy. The first, focusing on electron-transfer theory, was held at PacifiChem in 2021 having been delayed from 2020 owing to the Covid-19 pandemic and because of this, it was held purely online. With attendees coming from all time zones across the globe, this was a challenging but rewarding event. The second was held at the RACI National Convention in Brisbane in 2022 in a session on molecular electronics, highlighting Hush's development of the field. This was an exciting meeting in the end-of-Covid era that brought people together from all over Australia and also overseas. The Noel Hush Symposium fittingly at the University of Sydney was the third, and it was held in July 2024 in conjunction with the national meeting of the Physical Chemistry Division of the Royal Australian Chemical Institute. Speakers (the full programme is included in the Supplementary Material that accompanies this biographical memoir) described their association with Hush and his influence on the development of theoretical chemistry in Australia and internationally.

Tributes paid to Hush at the memorial service held in the Great Hall of the University of Sydney on 27 May 2019, and literary magazine *Quadrant*, with which he had been associated (see below), published a notice of his death, writing that he 'became one of the great scientists of his times' who was 'dedicated to the preservation of liberal and conservative values in Australian society'. *Quadrant* also included tributes from his colleagues, Max Bennett describing him as 'a really lovely man … held in near reverence at Sydney' and by Jeff Reimers who wrote that Hush's 'vision that 1 day molecules would replace silicon in electronic circuits … lives on' (Bennett and Reimers 2019).

Hush's scientific work was the subject of a chapter in *The Search for Knowledge and Understanding*, a book (Bennett 2019) commissioned by the Vice-Chancellor to commemorate the greatest scholars over the history of the University of Sydney. It was written by Max Bennett, Emeritus Professor of Neuroscience at Sydney, with whom Hush had lunched each month over many years. Bennett concluded his account with 'Hush has been and remains, at 94 years old, the greatest scientist at the University of Sydney. This perspective is based not only on his being elected to all the world's most prestigious societies and receiving the premier award in chemistry, The Welch Prize, but, more particularly, on the elegance of his penetrating analysis of electron transfer … that holds the key to understanding molecular reactions'.

Near the School of Chemistry at the University of Sydney, Hush is remembered by a memorial plinth (Fig. 5) on which he is described as a 'pioneer of electron transfer theory—the basis of molecular reactions'.

Fig. 5. Hush memorial plaque on the University of Sydney campus (Jeff Reimers).

Personal

Noel Hush and Thea Lesley, daughter of Leslie Harold and Mary Irene Warman, were married on 18 November 1949, soon after they arrived in Manchester. Thea had matriculated at the North Sydney Girls' High school and graduated BA from the University of Sydney in 1949. She was employed at different times in a variety of occupations that included working in a small art gallery, nightclub work, and teaching, but her real vocation was writing. Her career can be said to have begun at age twelve, when her article describing her family's drive to Narooma was published in the Sydney *Sun* (Warman 1937). Her novel *The Edifice* (Hush 1960), was published in London. On her return to Australia, Thea was a book reviewer for *The Australian* newspaper from 1972–8, and she continued writing, winning a Commonwealth writers' award and two state awards. In 1975 she completed another novel that was still undergoing final revision before publication when she died in 1978.

Two children were added to the Hush family in Bristol, David in 1956, and Julia in 1962. David included music among his studies at Clifton College in Bristol, but after completing his schooling in Sydney he completed the Arts component of an Arts/Law degree at the University of Sydney. Forsaking the possibility of furthering those studies at the University of Cambridge, however, he studied music at Sydney and moved to study twentieth- century music with Milton Babbitt at Princeton University in the United States, where he took his PhD. Returning to Australia in 1993, he has worked as a neo-classical composer, and joining his father, in 2018 he became a Fellow of the Royal Society of New South Wales.

Julia studied Plant Biophysics at the University of Sydney, earning a First Class Honours degree and a PhD. A Fulbright Award enabled her to undertake post-doctoral studies in Massachusetts, after which she returned to Australia to take up an ARC Fellowship. Before completing this, however, she decided to switch fields, enrolling as an undergraduate at the University of Sydney to study for a Bachelor of Applied Science in Physiotherapy. This led to a successful career as a physiotherapist until, eventually responding to the call of learning, she took up a lectureship in the School of Health Sciences at the University of Sydney. She was one of the founders of the Department of Health Sciences at Macquarie University, where she eventually was made full Professor, and specialised in the field of pain management.

Noel Hush was socially conservative, and served for twenty years as a member of the board of directors of the Australian literary magazine *Quadrant*, a journal that espouses as its 'principal purpose the defence of the values, practices, and institutions of a free and open society by fostering literary and cultural activity of the highest standard … and the preservation and advancement of the cultural freedom that is the distinctive component of traditional Western culture'.[6]

[6]https://quadrant.org.au/about-us/, viewed July 2025.

Supplementary material

Supplementary material is available online.

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Data availability. No data were created specifically for this biographical memoir.

Conflicts of interest. Jeffrey Reimers was a colleague and research collaborator of Hush for many years. Ian Rae is co-Editor-in-Chief of *Historical Records of Australian Science*. To mitigate this potential conflict of interest he had no editor-level access to this manuscript during peer review.

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