

Supplementary Material

Noel Sydney Hush (1924–2019)

Ian D. Rae^{A,*} and Jeffrey R. Reimers^{B,C}

^ASchool of Chemistry, University of Melbourne, Parkville, Vic 3010, Australia

^BInternational Centre for Quantum and Molecular Structures, Department of Physics, Shanghai University, Shanghai, 200444, China

^CSchool of Mathematical and Physical Sciences, University of Technology Sydney, 15 Broadway, Ultimo, NSW 2007, Australia

*Correspondence to: Email: iandrae@bigpond.com

BIOGRAPHICAL MEMOIR NOEL SYDNEY HUSH: SUPPLEMENTARY MATERIAL

Career outline

BSc (Sydney), 1946, with Honours in Organic Chemistry

MSc (Sydney), 1948

DSc (Manchester), 1959

1946–48 Held Dunlop Research Fellowship, University of Sydney

1948–49 Teaching Fellow in Chemistry, University of Sydney

1949–54 Assistant Lecturer in Physical Chemistry, University of Manchester

1954–63 Lecturer in Physical and Inorganic Chemistry, University of Bristol

1965–56 Theoretical Consultant, Ministry of Supply

1960–61 Visiting Research Fellow, Department of Theoretical Physics, Australian National University

1962–66 Visiting Scientist, Brookhaven National Laboratory, New York, July–Sept 1962 and Sep 1966

1963–71 Reader in Inorganic Chemistry, University of Bristol

1966–67 Visiting Professor, Institute of Biophysics, Florida State University, Oct 1966–March 1967

1969 Frontiers in Chemistry Lecturer and Visiting Professor, Case Western Reserve University, Cleveland, Ohio, March–April

1971 Professor of Theoretical Chemistry, University of Sydney

1989 Retirement, Emeritus in Chemistry, then affiliated with School of Molecular Biosciences, University of Sydney

Honours and awards

1977 Fellow of the Australian Academy of Science (FAA)

1977 Fellow of the Royal Australian Chemical Institute (FRACI)

1988 Fellow of the Royal Society (FRS)

1990 Centenary Medal of the Royal Society of Chemistry

1993 Officer of the Order of Australia (AO)

1994 Matthew Flinders Medal and Lecture from the Australian Academy of Science

1999 Foreign Member of the American Academy of Arts and Sciences

2000 Inaugural David Craig Medal and Lecture of the Australian Academy of Science

2001 Australian Federation Centenary Medal

2005 Physical Division Medal of the Royal Australian Chemical Institute (FRACI)

2007 Welch Award

2010 Fellow of the Royal Society of New South Wales (FRNS)

2011 Foreign Associate of the National Academy of Sciences of USA.

2014 Ahmed Zewail Prize for Molecular Science

Bibliography: Noel Sydney Hush

This bibliography lists extended conference abstracts and all peer-reviewed articles but not brief book reviews or short conference abstracts.

1947

Hughes, GK & Hush, NS (1947). Studies in semiquinones. Part I. P-phenylene diamine and benzidine derivatives. *Journal and Proceedings of the Royal Society of New South Wales* 81, 48–59.

Hughes, GK, Hush, NS & Mellor, DP (1947). Polymerization of a semiquinone ion. *Nature* 159, 612.

1948

Hush, NS (1948). The oxidation states of thallium. *Australian Journal of Science* 10, 184.

Hush, NS (1948). The free energies of hydration of gaseous ions. *Australian Journal of Scientific Research, Series A: Physical Sciences* 1, 480–493.

Hush, NS (1948). Disproportionation equilibria in alkaline earth ions. *Journal and Proceedings of the Royal Society of New South Wales* 82, 229–240.

1952

Evans, MG & Hush, NS (1952). Ionogenic reactions involving bond-breaking at electrodes. *Journal de Chimie Physique* 49, supplement 2, C159–171.

Evans, MG, Hush, NS & Uri, N (1952). The energetics of reactions involving hydrogen peroxide, its radicals, and its ions. *Quarterly Reviews of the Chemical Society* 6, 186–196.

Hush, NS (1952). The stability of semiquinones. *The Journal of Chemical Physics* 20, 1343–1344.

Hush, NS (1952). Reduction potentials and unsaturation energy changes in electrode reactions leading to the formation of acridyl radicals. *The Journal of Chemical Physics* 20, 1660–1661.

1953

Hush, NS (1953). Quantum-mechanical discussion of the gas-phase formation of quinonodimethide monomers. *Journal of Polymer Science* 11, 289–298.

Hush, NS (1953). The influence of conjugation on the ionization of aromatic amines. *Journal of the Chemical Society (Resumed)* 1953, 684–691.

Hush, NS (1953). The unsaturation energies of aroxyl radicals. *Journal of the Chemical Society (Resumed)* 1953, 2375–2380.

1955

Hush, NS & Blackledge, J (1955). Electron interaction in hydrocarbon multiple ions. *The Journal of Chemical Physics* 23, 514–517.

Hush, NS & Pople, JA (1955). Ionization potentials and electron affinities of conjugated hydrocarbon molecules and radicals. *Transactions of the Faraday Society* 51, 600–605. (This paper is reprinted in *The Quantum Theory of Molecular Electronic Structure*, 1963, ed. by RG Parr. W.A. Benjamin, New York).

1956

Hush, NS (1956). Phenate ion and the $\text{Fe}^{3+}\text{PhO}^-$ ion-pair complex. *Recueil des Travaux Chimiques des Pays-Bas* 75, 1101–1104.

Hush, NS (1956). Adiabatic electron-transfer, and contributions to discussion on electrode kinetics. *Fourth Moscow Symposium on Electrochemistry*, 1956. (English translation by Consultants Bureau, New York, 1961).

Hush, NS & Rowlands, JR (1956). Electronic spectra of hydrocarbon anions. *The Journal of Chemical Physics* 25, 1076–1077.

1957

Hush, NS (1957). Successive ionization potentials of unsaturated hydrocarbons. *The Journal of Chemical Physics* 27, 612–613.

Hush, NS (1957). Electrode reactions of the methyl halides. *Zeitschrift für Elektrochemie, Berichte der Bunsengellschaft für Physikalische Chemie* 61, 734–738.

Hush, NS (1957). The use of electronically-switched microelectrodes in the study of oxidation-reduction processes. *Zeitschrift für Elektrochemie, Berichte der Bunsengellschaft für Physikalische Chemie* 61, 738–744.

Hush, NS & Pryce, MHL (1957). Radii of transition ions in crystal fields. *The Journal of Chemical Physics* 26, 143–144.

1958

Hush, NS (1958). Adiabatic rate processes at electrodes. I. Energy-charge relationships. *The Journal of Chemical Physics* 28, 962–972.

Hush, NS (1958). Crystal-field stabilization and site deformation in crystals and complexes containing transition ions. *Discussions of the Faraday Society* 26, 145–156.

Hush, NS (1958). Theory of intensities of optical absorption bands in transition-metal complexes. *Bulletin of the Photoelectric Spectrometry Group* 11, 281.

Hush, NS & Pryce, MHL (1958). Influence of the crystal-field potential on interionic separation in salts of divalent iron-group ions. *The Journal of Chemical Physics* 28, 244–249.

1960

Hush, NS (1960). Contributions to discussions on electron transfer processes. *Discussions of the Faraday Society* 29, 113, 116, 133, 249.

1961

Hush, NS (1961). Adiabatic theory of outer sphere electron-transfer reactions in solutions. *Transactions of the Faraday Society* 57, 557–580.

1962

Dodd, JW, Hopton, FJ & Hush, NS (1962). Electronic spectra of aza-benzene anions. *Proceedings of the Chemical Society* 143, 61–62.

Hush, NS (1962). 7-coordinated transition complexes in inorganic substitution reactions. *Australian Journal of Chemistry* 15, 378–382.

1963

Blackledge, J & Hush, NS (1963). Mechanism of the $\text{Zn}^{2+}/\text{Zn}(\text{Hg})$ exchange: Part 2: catalysis by halide and thiocyanate ions. *Journal of Electroanalytical Chemistry* 5, 435–449.

Hopton, FJ & Hush, NS (1963). The electronic absorption spectrum of the benzyl anion. *Molecular Physics* 6, 209–213.

Hush, NS (1963). The function of bridging groups in electron-transfer reactions. *Brookhaven National Laboratory Publication* no. 6561.

Hush, NS & Blackledge, J (1963). Mechanism of the $\text{Zn}^{\text{II}}/\text{Zn}(\text{Hg})$ exchange: Part 1: the $\text{Zn}^{2+}/\text{Zn}(\text{Hg})$ exchange. *Journal of Electroanalytical Chemistry* 5, 420–434.

Hush, NS & Oldham, KB (1963). The electroreduction of organic iodides and organomercuric halides. *Journal of Electroanalytical Chemistry* 6, 34–45.

Hush, NS & Rowlands, JR (1963). The effect of alkali-metal ion association on the electronic spectra of the mononegative ions of naphthalene and anthracene. *Molecular Physics* 6, 201–208.

Hush, NS & Rowlands, JR (1963). The excited states of biphenylene and its negative and positive ions. *Molecular Physics* 6, 317–328.

1964

Dodd, JW & Hush, NS (1964). The negative ions of some porphin and phthalocyanine derivatives, and their electronic spectra. *Journal of the Chemical Society (Resumed)* 1964, 4607–4612.

Hush, NS & Scarrott, JW (1964). Kinetics of water exchange in the hydration shell of Ni^{2+} ion at a mercury-solution interface. *Journal of Electroanalytical Chemistry* 7, 26–37.

1965

Case, B, Hush, NS, Parsons, R & Peover, ME (1965). The real solvation energies of hydrocarbon ions in acetonitrile and the surface potential of acetonitrile. *Journal of Electroanalytical Chemistry* 10, 360–370.

Clack, DW & Hush, NS (1965). Successive one-electron reduction potentials of porphins and metal porphins in dimethylformamide. *Journal of the American Chemical Society* 87, 4238–4242.

1966

Hush, NS (1966). Ground-state energies of mono-, di-, tri- and tetranegative ions of porphins and their metal complexes. *Theoretica Chimica Acta (Berlin)* 4, 108–113.

1967

Allen, GC & Hush, NS (1967). Reflectance spectrum and electronic states of the CuCl_5^{3-} ion in a number of crystal lattices. *Inorganic Chemistry* 6, 4–8.

Allen, GC & Hush, NS (1967). Intervalence-transfer absorption. Part 1. Qualitative evidence for intervalence-transfer absorption in inorganic systems in solution and the solid state. Pages 357–389 in *Progress in Inorganic Chemistry*, ed. by FA Cotton. John Wiley & Sons, London.

Clack, DW, Hush, NS & Yandle, JR (1967). The electron spin resonance spectra of metal phthalocyanine negative ions. *Chemical Physics Letters* 1, 157–159.

Hush, NS (1967). Intervalence-transfer absorption. Part 2. Theoretical considerations and spectroscopic data. Pages 391–444 in *Progress in Inorganic Chemistry*, ed. by FA Cotton. John Wiley & Sons, London.

Hush, NS & Rowlands, JR (1967). Hyperfine structure in the electron spin resonance spectra of reduced porphins. *Journal of the American Chemical Society* 89, 2976–2979.

Hush, NS & Yandle, JR (1967). Calculation of dipole moments of some heterocyclic molecules by the CNDO molecular orbital method. *Chemical Physics Letters* 1, 493–494.

1968

- Hush, NS (1968). Homogeneous and heterogeneous optical and thermal electron transfer. *Electrochimica Acta* 13, 1005–1023.
- Hush, NS (1968). Contributions to discussions on electrode reactions. *Discussions of the Faraday Society* 45, 52, 56, 58, 59, 65, 176, 185.
- Hush, NS & Hobbs, RJM (1968). Absorption spectra of crystals containing transition metal ions. Pages 259–486 in *Progress in Inorganic Chemistry*, ed. by FA Cotton. John Wiley & Sons, London.
- Hush, NS & Segal, GA (1968). Semi-empirical SCF MO calculations of the electronic structures of CH_3F and CH_3F^- and their significance for adiabatic electrode processes involving bond-breaking. *Discussions of the Faraday Society* 45, 23–29.

1969

- Hush, NS, Dyke, JM, Williams, ML & Woolsey, IS (1969). Predicted bond lengths and π -electron distribution in the fully conjugated corrole ring. *Molecular Physics* 17, 559–560.

1970

- Hush, NS & Williams, ML (1970). Finite-perturbation SCF valence-shell calculations of molecular polarizability and hyperpolarizability components. *Chemical Physics Letters* 5, 507–510.
- Hush, NS & Williams, ML (1970). Finite electric field SCF calculations of molecular polarizabilities: absolute polarizabilities. *Chemical Physics Letters* 6, 163–165.

1971

- Dyke, JM, Hush, NS, Williams, ML & Woolsey, IS (1971). Bond lengths and location of the inner-ring protons in the corrole molecule. *Molecular Physics* 20, 1149–1152.
- Hush, NS (ed.) (1971). *Reactions of Molecules at Electrodes*. Wiley-Interscience, London.
- Hush, NS & Williams, ML (1971). Oscillator strengths in porphyrins. *Chemical Physics Letters* 8, 179–182.
- Hush, NS & Woolsey, IS (1971). The electronic absorption spectra of phthalocyanine monomers and dimers. *Molecular Physics* 21, 465–474.
- Linder, RE, Rowlands, JR & Hush, NS (1971). Magnetic circular dichroism and theoretical studies of the excited states of magnesium phthalocyanine negative ions. *Molecular Physics* 21, 417–437.

1972

- Clack, DW, Hush, NS & Yandle, JR (1972). All-valence electron CNDO calculations on transition metal complexes. *The Journal of Chemical Physics* 57, 3503–3510.
- Dyke JM & Hush, NS (1972). A spectroscopic study of Eu(III)/Eu(II) and Sm(III)/Sm(II) solutions in acetonitrile obtained by controlled-potential reduction. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry* 36, 337–347.
- Hush, NS & Williams, ML (1972). Finite electric field valence shell calculations of polarizability gradients and Raman depolarization ratios for diatomic molecules. *Theoretica Chimica Acta (Berlin)* 26, 141–146.
- Hush, NS & Williams, ML (1972). Finite electric field valence-shell calculations of molecular hyperpolarizabilities. *Theoretica Chimica Acta (Berlin)* 25, 346–351.
- Hush, NS & Woolsey, IS (1972). A study of the reduced species of cobalt and nickel complexes analogous to vitamin B₁₂. *Journal of the American Chemical Society* 94, 4107–4114.

1973

- Hush, NS & Dyke, JM (1973). A polarographic investigation of some metal tetrahydrocorrins. *Journal of Inorganic and Nuclear Chemistry* 35, 4341–4347.

1974

- Bacskey, GB & Hush, NS (1974). Molecules in electric fields I. The polarisability of the hydrogen molecule. *Theoretica Chimica Acta (Berlin)* 32, 311–320.
- Hush, NS & Dyke, JM (1974). Current-potential relationships in the reduction of samarium and europium perchlorates in dimethyl-formamide at a dropping mercury electrode. *Journal of Electroanalytical Chemistry and Interfacial Electrochemistry* 53, 253–260.
- Hush, NS, Dyke, JM, Williams, ML & Woolsey, IS (1974). Electronic spectra of metal corrole anions. *Journal of the Chemical Society, Dalton Transactions* 4, 395–399.
- Hush, NS & Williams, ML (1974). Carbon monoxide bond length, force constant and infrared intensity variations in strong electric fields: Valence-shell calculations, with applications to properties of adsorbed and complexed CO. *Journal of Molecular Spectroscopy* 50, 349–368.
- Hush, NS & Woolsey, IS (1974). Optical and electron spin resonance spectra of cobalt complexes related to vitamin B₁₂. *Journal of the Chemical Society, Dalton Transactions* 1, 24–34.

1975

- Hush, NS (1975). Inequivalent XPS binding energies in symmetrical delocalized mixed-valence complexes. *Chemical Physics* 10, 361–366.
- Hush, NS & Cheung, AS (1975). Ionization potentials and donor properties of nucleic acid bases and related compounds. *Chemical Physics Letters* 34, 11–13.
- Hush, NS, Cheung, AS & Hilton, PR (1975). Binding energies of π - and “lone-pair”-levels in mono- and diaza-phenanthrenes and anthracenes: an He(I) photoelectron spectroscopic study. *Journal of Electron Spectroscopy and Related Phenomena* 7, 385–400.

1976

- Bacskay, GB & Hush, NS (1976). Theoretical study of the N^+_2 molecular ion. *Chemical Physics* 16, 219–227.
- Beattie, JK, Hush, NS & Taylor, PR (1976). Electron delocalization in the mixed-valence μ -pyrazine-decaamminediruthenium(5+) ion. *Inorganic Chemistry* 15, 992–993.
- Clack, DW, Hush, NS & Woolsey, IS (1976). Reduction potentials of some metal phthalocyanines. *Inorganica Chimica Acta* 19, 129–132.
- Hilton, PR, Nordholm, S & Hush, NS (1976). Molecular photoionization cross sections calculated by an effective plane wave method. *Chemical Physics* 15, 345–361.
- Taylor, PR, Bacskay, GB, Hush, NS & Hurley, AC (1976). The coupled-pair approximation in a basis of independent-pair natural orbitals. *Chemical Physics Letters* 41, 444–449.

1977

- Beattie, JK, Hush, NS, Taylor, PR, Raston, CL & White, AH (1977). Crystal structure of μ -pyrazine-bis(penta-ammineruthenium) penta-(bromide chloride)-water (1/4). *Journal of the Chemical Society, Dalton Transactions* 11, 1121–1124.
- Gready, JE, Bacskay, GB & Hush, NS (1977). Finite-field method calculations of molecular polarisabilities. I. Theoretical basis and limitations of SCF and Galerkin treatments. *Chemical Physics* 22, 141–150.
- Gready, JE, Bacskay, GB & Hush, NS (1977). Finite-field method calculations of molecular polarisabilities. II. Theoretical analysis of the correlation corrections with application to some pseudo-two-electron systems. *Chemical Physics* 23, 9–22.
- Gready, JE, Bacskay, GB & Hush, NS (1977). Finite-field method calculations. III. Dipole moment gradients, polarisability gradients and field-induced shifts in bond lengths,

- vibrational levels, spectroscopic constants and dipole functions - application to lithium hydride. *Chemical Physics* 24, 333–341.
- Hilton, PR, Nordholm, S & Hush, NS (1977). The ground state inversion potential method: application to the calculation of photoionization cross sections. *The Journal of Chemical Physics* 67, 5213–5223.
- Hush, NS & Cheung, AS (1977). Study of valence-level splitting in a porphin-type π -cation dimer by He(I) photoelectron spectroscopy. *Chemical Physics Letters* 47, 1–4.
- Hush, NS & Süzer, S (1977). Satellite structure in the atomic UV photoelectron spectra of Zn, Cd, and Hg observed at different wavelengths. *Chemical Physics Letters* 46, 411–414.
- Süzer, S, Hilton, PR, Hush, NS & Nordholm, S (1977). UV Subshell photoionisation cross-section of atomic Zn, Cd, and Hg: experiment and theory. *Journal of Electron Spectroscopy and Related Phenomena* 12, 357–374.
- Süzer, S & Hush, NS (1977). Satellites in the 304 AA photoelectron spectrum of Xe. *Journal of Physics B: Atomic and Molecular Physics* 10, L705.

1978

- Cribb, PH, Nordholm, S & Hush, NS (1978). Calculation of tunnelling and over-barrier decay rates by a generalised method of beats. *Chemical Physics* 29, 31–41.
- Cribb, PH, Nordholm, S & Hush, NS (1978). Theory of unimolecular reactions in one dimension. *Chemical Physics* 29, 43–54.
- Gready, JE, Bacskay, GB & Hush, NS (1978). Comparison of multipole moment expansions by direct summation or finite-field SCF methods with full electrostatic interaction energies: application to CO and N₂. *Chemical Physics* 31, 375–390.
- Gready, JE, Bacskay, GB & Hush, NS (1978). Finite-field method calculations. IV. Higher-order moments, dipole moment gradients, polarisability gradients and field-induced shifts in molecular properties: application to N₂, CO, CN⁻, HCN and HNC. *Chemical Physics* 31, 467–483.
- Gready, JE, Bacskay, GB & Hush, NS (1978). Calculation of electrostatic interaction energies in physisorption studies of ionic surfaces. *Journal of the Chemical Society, Faraday Transactions 2*, 1430–1440.
- Taylor, PR, Bacskay, GB, Hush, NS & Hurley, AC (1978). Unlinked cluster effects in molecular electronic structure. I. The HCN and HNC molecules. *The Journal of Chemical Physics* 69, 1971–1979.

Taylor, PR, Bacskay, GB, Hush, NS & Hurley, AC (1978). Unlinked cluster effects in molecular electronic structure. II. Pair correlations in the molecules HCN and HNC. *The Journal of Chemical Physics* 69, 4669–4677.

1979

Cribb, PH, Nordholm, S & Hush, NS (1979). A density matrix approach to double well transfer: effects of asymmetry on the tunneling rate. *Chemical Physics* 44, 315–335.

Cribb, PH, Nordholm, S & Hush, NS (1979). A general theoretical approach to tunneling transfer and dissociation. Pages 139–144 in *Tunneling in Biological Systems*, ed. by B Chance, DC Devault, H Frauenfelder, RA Marcus, JR Schrieffer & N Sutin. Academic Press, New York.

Gready, JE, Bacskay, GB & Hush, NS (1979). On the absolute signs of the CH and CN dipole moment derivatives of HCN. *The Journal of Chemical Physics* 70, 1071–1072.

Hilton, PR, Nordholm, S & Hush, NS (1979). Photoionization cross section of water by an atomic extrapolation method. *Chemical Physics Letters* 64, 515–518.

Hush, NS, Hilton, PR & Nordholm, S (1979). Calculation of atomic and molecular photoionization cross sections using the ground state inversion potential method. *Journal of Electron Spectroscopy and Related Phenomena* 15, 101–107.

John, IG, Bacskay, GB & Hush, NS (1979). Finite field method calculations. V. Raman scattering activities and infrared absorption intensities for H₂O, D₂O, CH₄ and CD₄. *Chemical Physics* 38, 319–328.

Taylor, PR, Bacskay, GB, Hush, NS & Hurley, AC (1979). Unlinked cluster effects in molecular electronic structure. III. Potential curve for the CN⁻ ion and the adiabatic electron affinity of CN. *The Journal of Chemical Physics* 70, 4481–4490.

1980

Cribb, PH, Nordholm, S & Hush, NS (1980). The role of tunnelling in light atom diffusion in metals: a comparison of *resonant* and *non-resonant* theoretical approaches. *Chemical Physics* 47, 135–147.

Hilton, PR, Nordholm, S & Hush, NS (1980). Ground-state inversion method applied to calculation of molecular photoionization cross-sections by atomic extrapolation: interference effects at low energies. *Journal of Electron Spectroscopy and Related Phenomena* 18, 101–119.

Hush, NS (1980). Electron delocalization, structure and dynamics in mixed-valence systems. Pages 151–188 in *Mixed-Valence Compounds*, ed. by DB Brow. D Reidel Publishing Co., Dordrecht.

Hush, NS (1980). On the calculation of intensities of molecular vibrational transitions and of Raman scattering due to molecular vibrations. Pages 1.7.1–1.7.24 in *Molecular Physics and Quantum Chemistry: into the 80's*. Workshop on molecular physics and quantum chemistry, Wollongong, February 1980. University of Wollongong, Wollongong.

Hush, NS, Edgar, A & Beattie, JK (1980). Single-crystal EPR study of a mixed-valence ruthenium dimer ion: the ground state of the Creutz-Taube complex. *Chemical Physics Letters* 69, 128–133.

John, IG, Bacskay, GB & Hush, NS (1980). Finite field method calculations. VI. Raman scattering activities, infrared absorption intensities and higher-order moments: SCF and CI calculations for the isotopic derivatives of H₂O and SCF calculations for CH₄. *Chemical Physics* 51, 49–60.

Taylor, PR, Bacskay, GB, Hush, NS & Hurley, AC (1980). Unlinked cluster effects in molecular electronic structure. Pages 1.3.1–1.3.22 in *Molecular Physics and Quantum Chemistry: into the 80's*. Workshop on molecular physics and quantum chemistry, Wollongong, February 1980. University of Wollongong, Wollongong.

1982

Cribb, PH, Nordholm, S & Hush, NS (1982). A comparison of tunneling transfer theories for asymmetric isomerization reactions. *Chemical Physics* 69, 259–266.

Gready, JE, Bacskay, GB & Hush, NS (1982). Comparison of the effects of symmetric versus asymmetric H bonding on ²H and ¹⁷O nuclear quadrupole coupling constants: application to formic acid and the hydrogen diformate anion. *Chemical Physics* 64, 1–17.

Hush, NS (1982). Parameters of electron-transfer kinetics. Pages 301–332 in *Mechanistic Aspects of Inorganic Reactions*, ed. by DB Rorabacher & JF Endicott. American Chemical Society Symposium Series 198, Washington, D.C.

1983

Hush, NS (1983). Thermal and optical electron transfer probabilities in biological systems. *Inorganica Chimica Acta* 79, 55.

Swanton, DJ, Bacskay, GB & Hush, NS (1983). An *ab initio* SCF calculation of the dipole-moment derivatives and infrared-absorption intensities of the water-dimer molecule. *Chemical Physics* 82, 303–315.

Swanton, DJ, Bacskay, GB, Willett, GD & Hush, NS (1983). Structure and relative stabilities of isomers of $C_2H_2N^+$: an *ab initio* molecular orbital study. *Journal of Molecular Structure: Theochem* 91, 313–323.

1984

Armstrong, RS, Beattie, JK, del Favero, P, Ellis, VM & Hush, NS (1984). Electronic and resonance Raman spectroscopic evidence for identification of μ -trihalobi(triammine-ruthenium)(2+) ions as delocalized Ru(II,III) mixed-valence complexes. *Inorganica Chimica Acta* 89, L33–L34.

Hush, NS, Beattie, JK & Ellis, VM (1984). Electronic spectra of tris(μ -halo)bis(triammineruthenium)(2+) ions: evidence for delocalized mixed-valence D_{3h} Ru(II,III) ground states. *Inorganic Chemistry* 23, 3339–3342.

Swanton, DJ, Bacskay, GB & Hush, NS (1984). An *ab initio* SCF calculation of the polarizability tensor, polarizability derivatives and Raman scattering activities of the water- dimer molecule. *Chemical Physics* 83, 69–75.

1985

Cummins, PL, Bacskay, GB & Hush, NS (1985). *Ab initio* quantum chemical studies of electric field gradients in the hydrogen-bonded N_2 –HF and N_2 –HCl complexes. *The Journal of Physical Chemistry* 89, 2151–2155.

Cummins, PL, Bacskay, GB, Hush, NS, Halle, B & Engström, S (1985). The effect of intermolecular interactions on the 2H and ^{17}O quadrupole coupling constants in ice and liquid water. *The Journal of Chemical Physics* 82, 2002–2013.

Hush, NS (1985). Distance dependence of electron transfer rates. *Coordination Chemistry Reviews* 64, 135–157.

Hush, NS, Paddon-Row, MN, Cotsaris, E, Oevering, H, Verhoeven, JW & Heppener, M. (1985). Distance dependence of photoinduced electron transfer through non-conjugated bridges. *Chemical Physics Letters* 117, 8–11.

Rendell, APL, Bacskay, GB & Hush, NS (1985). The validity of electrostatic predictions of the shapes of van der Waals dimers. *Chemical Physics Letters* 117, 400–408.

1986

Cummins, PL, Rendell, APL, Swanton, DJ, Bacskay, GB & Hush, NS (1986). The role of electrostatics in molecular interactions: prediction of shapes and electronic properties of weakly bound complexes. *International Reviews in Physical Chemistry* 5, 139–146.

- Hush, NS, Willett, GD, Paddon-Row, MN, Patney, HK & Peel, JB (1986). Orbital interactions. Part 13. The observation of through-bond orbital interactions between benzene and double bonds in some dimethanoanthracenes. *Journal of the Chemical Society, Perkin Transactions 2*, 827–833.
- Kilcoyne, DAL, McCarthy, CM, Nordholm, S, Hush, NS & Hilton, PR (1986). An atomic diffraction theory of molecular photoionization cross sections. *Journal of Electron Spectroscopy and Related Phenomena* 36, 153–185.
- Kilcoyne, DAL, Nordholm, S & Hush, NS (1986). Analysis of photoionisation cross sections of molecular fluorine and chlorine, and hydrogen chloride by a pseudo-atomic diffraction theory: interference enhancement and its dependence on orbital type. *Chemical Physics* 107, 197–212.
- Kilcoyne, DAL, Nordholm, S & Hush, NS (1986). Diffraction analysis of the photoionisation cross sections of water, ammonia and methane. *Chemical Physics* 107, 213–223.
- Kilcoyne, DAL, Nordholm, S & Hush, NS (1986). An analysis of photoionisation cross sections for carbon monoxide and dioxide and nitrous oxide by diffraction theory. *Chemical Physics* 107, 225–253.
- Kilcoyne, DAL, Nordholm, S & Hush, NS (1986). Photoionisation of ethylene and benzene: a theoretical analysis of multicentre diffraction effects. *Chemical Physics* 107, 255–282.
- Swanton, DJ, Bacskay, GB & Hush, NS (1986). A quantum chemical study of the infrared absorption intensities of the isoelectronic C_{3v} systems NH_3 , H_3O^+ and CH_3^- . *Chemical Physics* 107, 9–23.
- Swanton, DJ, Bacskay, GB & Hush, NS (1986). A quantum chemical study of the infrared absorption intensities of the isoelectronic C_{2v} systems H_2F^+ , H_2O and NH_2^- . *Chemical Physics* 107, 25–31.
- Swanton, DJ, Bacskay, GB & Hush, NS (1986). The infrared absorption intensities of the water molecule: a quantum chemical study. *The Journal of Chemical Physics* 84, 5715–5727.
- Warman, JM, de Haas, MP, Oevering, H, Verhoeven, JW, Paddon-Rowe, MN, Oliver, AM & Hush, NS (1986). Donor, acceptor, and self-quenching of the giant-dipole state of a rigid, σ -bond separated, donor-acceptor molecular assembly. *Chemical Physics Letters* 128, 95–99.
- Warman, JM, de Haas, MP, Paddon-Rowe, MN, Cotsaris, E, Hush, NS, Oevering, H & Verhoeven, JW (1986). Light-induced giant dipoles in simple model compounds for photosynthesis. *Nature* 320, 615–616.

- Bacskay, GB, Bryant, G & Hush, NS (1987). Hole localization and broken symmetry: a theoretical study of core electron ionization in the Li₂ molecule. *International Journal of Quantum Chemistry* 31, 471–487.
- Cummins, PL, Bacskay, GB & Hush NS (1987). *Ab initio* quantum chemical studies of the electronic properties of the hydrogen bonded N₂–HF, N₂–HCl, (HCN)₂ and NH₃–HCN complexes. *Chemical Physics* 115, 325–337.
- Cummins, PL, Bacskay, GB & Hush NS (1987). The effects of intermolecular interactions on the electric field gradients in ice and liquid water. *Molecular Physics* 61, 795–811.
- Cummins, PL, Bacskay, GB & Hush NS (1987). The effect of intermolecular interactions on the electric field gradients in solid ammonia, tetrazole and imidazole. *Molecular Physics* 62, 193–213.
- Cummins, PL, Bacskay, GB & Hush NS (1987). The prediction of nuclear quadrupole moments from *ab initio* quantum chemical studies on small molecules. II. The electric field gradients at the ¹⁷O, ³⁵Cl, and ²H nuclei in CO, NO⁺, OH[–], H₂O, CH₂O, HCl, LiCl, and FCl. *The Journal of Chemical Physics* 87, 416–423.
- Cummins, PL, Bacskay, GB, Hush, NS & Ahlrichs, R (1987). The prediction of nuclear quadrupole moments from *ab initio* quantum chemical studies on small molecules. I. The electric field gradients at the ¹⁴N and ²H nuclei in N₂, NO, NO⁺, CN, CN[–], HCN, HNC, and NH₃. *The Journal of Chemical Physics* 86, 6908–6917.
- Hush, NS (1987). Photoinduced electron transfer through long rigid non-conjugated bridges: theory and experiment for model systems. Pages 53–72 in *Supramolecular Photochemistry*, ed. by V Balzani. D Reidel Publishing Co., Dordrecht.
- Hush, NS (1987). Report on the general discussion on "Future Trends: theoretical aspects". Pages 455–458 in *Supramolecular Photochemistry*, ed. by V Balzani. D Reidel Publishing Co., Dordrecht.
- Hush, NS, Livett, MK, Peel, JB & Willett, GD (1987). Variable-temperature ultraviolet photoelectron-spectroscopy of the keto-enol tautomers of pentane-2,4-dione. *Australian Journal of Chemistry* 40, 599–609.
- Oevering, H, Paddon-Row, MN, Heppener, M, Oliver, AM, Cotsaris, E, Verhoeven, JW & Hush, NS (1987). Long-range photoinduced through-bond electron transfer and radiative recombination via rigid nonconjugated bridges: distance and solvent dependence. *Journal of the American Chemical Society* 109, 3258–3269.

Rendell, APL, Bacskay, GB & Hush, NS (1987). An *ab initio* quantum chemical study of the hydrogen- and “anti”-hydrogen-bonded HF/ClF and HF/Cl₂ dimers. *The Journal of Chemical Physics* 87, 535–544.

Rendell, APL, Bacskay, GB, Hush, NS & Handy, NC (1987). The analytic configuration interaction gradient method: the calculation of one electron properties. *The Journal of Chemical Physics* 87, 5976–5986.

1988

Bacskay, GB, Rendell, APL & Hush, NS (1988). *Ab initio* quantum chemical study of the molecular and spectroscopic (infrared and Raman) properties of sulfur dioxide: comparison with ozone. *The Journal of Chemical Physics* 89, 5721–5730.

Beattie, JK, Del Favero, P, Hambley, TW & Hush, NS (1988). Crystal and molecular structure of the mixed-valence ruthenium dimer tris(μ -bromo)bis(triammineruthenium)(2+) tetrabromozincate(II), [(NH₃)₃RuBr₃Ru(NH₃)₃](ZnBr₄). *Inorganic Chemistry* 27, 2000–2002.

Cummins, PL, Bacskay, GB, Hush, NS & Jönsson, B. (1988). On the structure, lattice energy and ¹⁴N nuclear quadrupole coupling constant of solid HCN. *Chemical Physics Letters* 145, 399–406.

Oevering, H, Verhoeven, JW, Paddon-Row, MN, Cotsaris, E & Hush, NS (1988). Long-range exchange contribution to singlet-singlet energy transfer in a series of rigid bichromophoric molecules. *Chemical Physics Letters* 143, 488–495.

Oevering, H, Verhoeven, JW, Paddon-Row, MN, Cotsaris, E & Hush, NS (1988). On a long-range mechanism for energy-transfer in rigid bichromophoric molecules - reply. *Chemical Physics Letters* 150, 179–180.

Rendell, APL, Bacskay, GB & Hush, NS (1988). Electron transfer via dithiaspiroalkane linkages. Nature of long-range through-bond electronic coupling in disulfoxide radical cations and bis(metal) complexes and implications for the characterization of the SO bond. *Journal of the American Chemical Society* 110, 8343–8354.

1989

Reimers, JR & Hush, NS (1989). Electron transfer and energy transfer through bridged systems. I. Formalism. *Chemical Physics* 134, 323–354.

1990

Bacskay, GB, Kerdraon, DI & Hush, NS (1990). Quantum chemical study of the HCl molecule and its binary complexes with CO, C₂H₂, C₂H₄, PH₃, H₂S, HCN, H₂O and NH₃:

- hydrogen bonding and its effect on the ^{35}Cl nuclear quadrupole coupling constant. *Chemical Physics* 144, 53–69.
- Hush, NS, Wong, AT, Bacskay, GB & Reimers, JR (1990). Electron and energy transfer through bridged systems. 6. Molecular switches: the critical field in electric field activated bistable molecules. *Journal of the American Chemical Society* 112, 4192–4197.
- Reimers, JR & Hush, NS (1990). Formalism for electron transfer and energy transfer in bridged systems. Pages 27–63 in *Electron Transfer in Biology and the Solid State: inorganic compounds with unusual properties*, ed. by MK Johnson, RB King, DM Kurtz Jr, C Kutal, ML Norton & RA Scott. American Chemical Society, Washington, D.C.
- Reimers, JR & Hush, NS (1990). Spectroscopic evidence for electronically forbidden but vibronically allowed long-range electron transfer in norbornylog-bridged naphthalene-diacetyanoethylene systems. *Chemical Physics* 146, 105–114.
- Reimers, JR & Hush, NS (1990). Electron transfer and energy transfer through bridged systems. II. Tight binding linkages with zero asymptotic band gap. *Chemical Physics* 146, 89–103.
- Reimers, JR & Hush, NS (1990). Electron transfer and energy transfer through bridged systems. 4. Intermetallic coupling and electronic spectra of the bis(pentaammineruthenium) complexes of α,ω -dipyridyl *trans*-polyenes in nitrobenzene. *Inorganic Chemistry* 29, 4510–4513.
- Reimers, JR & Hush, NS (1990). Electron transfer and energy transfer through bridged systems. 5. Intermetallic coupling and electronic spectra of the bis(pentaammineruthenium) complexes of α,ω -dipyridyl *trans*-polyenes in D_2O . *Inorganic Chemistry* 29, 3686–3697.
- Reimers, JR, Hush, NS, Sammeth, DM & Callis, PR (1990). Two-photon fluorescence excitation spectrum of a naphthalene norbornylog: implications for electron transfer. *Chemical Physics Letters* 169, 622–626.

1991

- Bacskay, GB, Hush, NS & Ikuta, S (1991). Crowded molecules and “counterintuitive” substituent separations: quantum chemical calculations of equilibrium geometries and energies of 1,8-dichloro- and 1,4,5,8-tetrachloronaphthalene and 4,5-dichlorophenanthrene. *Journal of Physical Chemistry* 95, 9291–9297.
- Binstead, RA, Crossley, MJ & Hush, NS (1991). Modulation of valence orbital levels of metalloporphyrins by β -substitution: evidence from spectroscopic and electrochemical studies of 2-substituted metallo-5,10,15,20-tetraphenylporphyrins. *Inorganic Chemistry* 30, 1259–1264.

Hush, NS (1991). Electron tunnelling in chemistry: chemical reactions over large distances. In *Comprehensive Chemical Kinetics*, volume 30, ed. by RG Compton. Elsevier, Amsterdam.

Reimers, JR & Hush, NS (1991). Electric field perturbation of electronic (vibronic) absorption envelopes: application to characterization of mixed-valence states. Pages 29–50 in *Mixed Valency Systems: applications in chemistry, physics and biology*, ed. by K Prassides. Kluwer Academic Publishers, Amsterdam.

Reimers, JR & Hush, NS (1991). Electronic properties of transition-metal complexes determined from electroabsorption (Stark) spectroscopy. 2. Mononuclear complexes of ruthenium(II). *The Journal of Physical Chemistry* 95, 9773–9781.

Wong, AT, Bacskay, GB, Hush, NS & Bogaard, MP (1991). *Ab initio* polarizability derivatives for methane: an application to Raman intensities of overtone and combination bands. *Molecular Physics* 74, 1037–1064.

1992

Craw, JS, Hush, NS, Sternhell, S & Tansey, CW (1992). The relationship between partial bond fixation induced by through-bond and/or through-space perturbations in nonplanar benzene derivatives and ^1H spin–spin coupling constants. *Journal of Physical Chemistry* 96, 5753–5759.

Craw, JS, Reimers, JR, Bacskay, GB, Wong, AT & Hush, NS (1992). Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. I. Geometry. *Chemical Physics* 167, 77–99.

Craw, JS, Reimers, JR, Bacskay, GB, Wong, AT & Hush, NS (1992). Solitons in finite- and infinite-length negative-defect trans-polyacetylene and the corresponding Brooker (polymethinecyanine) cations. II. Charge density wave. *Chemical Physics* 167, 101–109.

Reimers, JR, Craw, JS & Hush, NS (1992). Soliton, charge-density wave structure and band gaps in odd polyene and symmetrical polymethinecyanine (Brooker) ions and in t-polyacetylene: implications for molecular electronics. *AIP Conference Proceedings* 262, 11–27.

1993

Binstead, RA & Hush, NS (1993). Hole localization and spin coupling in π -mono- and π -dications of μ -oxoporphyrin dimers. Relevance to structure of oxidized “special pair” in photosynthetic reaction centers. *The Journal of Physical Chemistry* 97, 13172–13179.

- Craw, JS, Bacskay, GB & Hush, NS (1993). Near doubling of H–H bond length in the “stretched” osmium molecular hydrogen complex $[\text{Os}(\text{NH}_3)\eta^2\text{-H}_2]^+$: a theoretical study. *Inorganic Chemistry* 32, 2230–2231.
- Reimers, JR, Craw, JS & Hush, NS (1993). Relation between predicted soliton charge-density wave structure of odd polyene anions and ^{13}C NMR chemical shifts. *The Journal of Physical Chemistry* 97, 2778–2787.
- Reimers, JR, Craw, JS, Wong, A, Bacskay, GB & Hush, NS (1993). Comparison of soliton geometry and charge-density wave structure, and band gaps, between odd polyene and symmetrical polymethine cyanine (Brooker) ions and t-polyacetylene: Sscf and model Hamiltonian approaches with implications for molecular wires and switches. *Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals* 234, 51–57.
- Reimers, JR & Hush, NS (1993). Hole, electron and energy transfer through bridged systems. VIII. Soliton molecular switching in symmetry-broken Brooker (polymethinecyanine) cations. *Chemical Physics* 176, 407–420.
- Zeng, J, Craw, JS, Hush, NS & Reimers, JR (1993). Solvent effects on molecular spectra. I. Normal pressure and temperature Monte Carlo simulations of the structure of dilute pyrimidine in water. *The Journal of Chemical Physics* 99, 1482–1495.
- Zeng, J, Craw, JS, Hush, NS & Reimers, JR (1993). Medium effects on molecular and ionic electronic spectra. Application to the lowest $^1(n, \pi^*)$ state of dilute pyridine in water. *Chemical Physics Letters* 206, 323–328.
- Zeng, J, Hush, NS & Reimers, JR (1993). Solvent effects on molecular spectra. II. Simulations of hydrated clusters and dilute solutions of pyrimidine in its lowest (n, π^*) singlet excited state. *The Journal of Chemical Physics* 99, 1496–1507.
- Zeng, J, Hush, NS & Reimers, JR (1993). Solvent effects on molecular spectra. III. Absorption to and emission from the lowest singlet (n, π^*) state of dilute pyrimidine in water. *The Journal of Chemical Physics* 99, 1508–1521.
- Zeng, J, Hush, NS & Reimers, JR (1993). Enthalpy of hydration and partial molar specific volume as criteria for evaluation of intermolecular potentials. NPT-ensemble Monte Carlo calculations for dilute neon in water. *Chemical Physics Letters* 206, 318–322.

1994

- Craw, JS, Bacskay, GB & Hush, NS (1994). Stretched molecular hydrogen complexes of osmium(II): a quantum chemical study of the influence of the *trans* ligand on geometries, spin-spin coupling constants, bonding, and charge distributions. *Journal of the American Chemical Society* 116, 5937–5948.

- Lü, TX, Reimers, JR, Crossley, MJ & Hush, NS (1994). Rigid fused oligoporphyrins as potential versatile molecular wires. 1. Geometry and connectivity of 1,4,5,8-tetraazaanthracene-bridged systems. *The Journal of Physical Chemistry* 98, 11878–11884.
- Reimers, JR & Hush, NS (1994). Electron transfer and energy transfer through bridged systems III. Tight-binding linkages with zero or non-zero asymptotic band gap. *Journal of Photochemistry and Photobiology A: Chemistry* 82, 31–46.
- Reimers, JR & Hush, NS (1994). The influence of spin-forbidden monomer excitations on spin-allowed electron transfer and electron-localized states of mixed-valence and single-valence dimeric systems. *Inorganica Chimica Acta* 226, 33–42.
- Zeng, J, Craw, JS, Hush, NS & Reimers, JR (1994). Solvent effects on molecular and ionic spectra. 4. Photochemistry of $\text{Fe}^{2+}(\text{H}_2\text{O})_6$ in water revisited: possible mechanisms for the primary absorption process leading to electron ejection. *The Journal of Physical Chemistry* 98, 11075–11088.

1995

- Hush, NS & Reimers, JR (1995). Vibrational Stark spectroscopy. 1. Basic theory and application to the CO stretch. *The Journal of Physical Chemistry* 99, 15798–15805.
- Reimers, JR, Craw, JS, Bacskay, GB & Hush, NS (1995). Towards efficient molecular wires and switches: the Brooker ions. *Biosystems* 35, 107–111.
- Reimers, JR & Hush, NS (1995). The nature of the near-infrared electronic absorption at 1250 nm in the spectra of the radical cations of the special pairs in the photosynthetic reaction centers of *Rhodobacter sphaeroides* and *Rhodospseudomonas viridis*. *Journal of the American Chemical Society* 117, 1302–1308.
- Reimers, JR & Hush, NS (1995). Nature of the ground and first excited states of the radical cations of photosynthetic bacterial reaction centres. *Chemical Physics* 197, 323–332.
- Reimers, JR, Lü, TX, Crossley, MJ & Hush, NS (1995). The mechanism of inner-hydrogen migration in free base porphyrin: *ab initio* MP2 calculations. *Journal of the American Chemical Society* 117, 2855–2861.
- Zeng, J, Hush, NS & Reimers, JR (1995). Solvent effects on molecular and ionic spectra. 5. Development of a method for simulation of the liquid structure and solvatochromic shift of inorganic complexes such as pentaaminopyridylruthenium(II) in water. *Journal of Physical Chemistry* 99, 10459–10470.
- Zeng, J, Woywod, C, Hush, NS & Reimers, JR (1995). Solvent effects on molecular and ionic spectra. 6. Hydrogen bonding and the delocalized nature of the first $^1(n,\pi^*)$ excited state of pyrazine. *Journal of the American Chemical Society* 117, 8618–8626.

1996

- Bacskay, GB, Bytheway, I & Hush, NS (1996). H–D spin–spin coupling in stretched molecular hydrogen complexes of osmium(II): density functional studies of *J_{HD}*. *Journal of the American Chemical Society* 118, 3753–3756.
- Bytheway, I, Bacskay, GB & Hush, NS (1996). Quantum chemical study of the properties of molecular hydrogen complexes of osmium(II): a comparison of density functional and conventional *ab initio* methods. *The Journal of Physical Chemistry* 100, 6023–6031.
- Bytheway, I, Bacskay, GB & Hush, NS (1996). Ligand exchange reactions in molecular hydrogen complexes of osmium(II): a quantum chemical study using density functional theory. *The Journal of Physical Chemistry* 100, 14899–14903.
- Reimers, JR & Hush, NS (1996). The effects of couplings to symmetric and antisymmetric modes and minor asymmetry on the spectral properties of mixed-valence and related charge-transfer systems. *Chemical Physics* 208, 177–193.
- Reimers, JR & Hush, NS (1996). Analytic solutions to resonant and non-resonant through-bridge electronic coupling. *Nanotechnology* 7, 417.
- Reimers, JR, Lü, TX, Crossley, MJ & Hush, NS (1996). Molecular electronic properties of fused rigid porphyrin-oligomer molecular wires. *Chemical Physics Letters* 256, 353–359.
- Reimers, JR, Zeng, J & Hush, NS (1996). Vibrational Stark spectroscopy. 2. Application to the CN stretch in HCN and acetonitrile. *The Journal of Physical Chemistry* 100, 1498–1504.
- Zeng, J, Hush, NS & Reimers, JR (1996). Solvent effects on molecular and ionic spectra. 7. Modeling the absorption and electroabsorption spectra of pentaammine-ruthenium(II) pyrazine and its conjugate acid in water. *Journal of the American Chemical Society* 118, 2059–2068.
- Zeng, J, Hush, NS & Reimers, JR (1996). Solvent effects on molecular and ionic spectra. VIII. The $^1(n,\pi^*)$ excited states of pyridazine in water. *The Journal of Physical Chemistry* 100, 9561–9567.
- Zeng, J, Hush, NS & Reimers, JR (1996). Solvent effects on molecular and ionic spectra IX: The change in dipole moment accompanying metal to ligand charge transfer absorption in pentaaminopyridylruthenium(II). *The Journal of Physical Chemistry* 100, 19292–19294.

1997

- Bytheway, I, Craw, JS, Bacskay, GB & Hush, NS (1997). Structure and bonding in molecular hydrogen complexes of osmium(II). Pages 21–38 in *Electron Transfer Reactions*:

- inorganic, organometallic, and biological applications*, ed. by SS Isied. American Chemical Society, volume 253, Washington, D.C.
- Hush, NS (1997). Relationship between H–D spin–spin coupling and internuclear distance in molecular hydrogen complexes. *Journal of the American Chemical Society* 119, 1717–1719.
- Hush, NS & Ulstrup, J (1997). Some historical notes on chemical charge transfer. Pages 1–24 in *Electron and Ion Transfer in Condensed Media: theoretical physics for reaction kinetics*, ed. by AA Kornyshev, M Tosi & J Ulstrup. World Scientific Publishing Co., Singapore.
- Reimers, JR & Hush, NS (1997). Molecular wires: operational principles and applications. Pages 326–346 in *Electron and Ion Transfer in Condensed Media: theoretical physics for reaction kinetics*, ed. by AA Kornyshev, M Tosi & J Ulstrup. World Scientific Publishing Co., Singapore.

1998

- Hush, NS & Reimers, JR (1998). Solvent effects on metal to ligand charge transfer excitations. *Coordination Chemistry Reviews* 177, 37–60.
- Hush, NS, Reimers, JR, Hall, LE, Johnston, LA & Crossley, MJ (1998). Optimization and chemical control of porphyrin-based molecular wires and switches. *Annals of the New York Academy of Sciences* 852, 1–21.
- Hush, NS, Zeng, J, Reimers, JR & Craw, JS (1998). The primary process in photooxidation of $\text{Fe}^{2+}(\text{H}_2\text{O})_6$ in water. Pages 263–277 in *Photochemistry and Radiation Chemistry: complementary methods for the study of electron transfer*, ed. by JF Wishart & DG Nocera. American Chemical Society, volume 254, Washington, D.C.
- Hutter, MC, Hughes, JM, Reimers, JR & Hush, NS (1998). Modeling the bacterial photosynthetic reaction center. 2. A combined quantum mechanical/molecular mechanical study of the structure of the cofactors in the reaction centers of purple bacteria. *The Journal of Physical Chemistry B* 103, 4906–4915.
- Hutter, MC, Reimers, JR & Hush, NS (1998). Modeling the bacterial photosynthetic reaction center. 1. Magnesium parameters for the semiempirical AM1 method developed using a genetic algorithm. *The Journal of Physical Chemistry B* 102, 8080–8090.
- Reimers, JR, Hall, LE, Hush, NS & Silverbrook, K (1998). Chemical control of tautomerization-based molecular electronic and color switches. *Annals of the New York Academy of Sciences* 852, 38–53.

Reimers, JR, Hutter, MC & Hush, NS (1998). The spectroscopy of the low-lying bands in the special-pair radical-cations of photosynthetic reaction centres. *Photosynthesis Research* 55, 163–171.

1999

Hush, NS (1999). Electron transfer in retrospect and prospect: 1: Adiabatic electrode processes. *Journal of Electroanalytical Chemistry* 470, 170–195.

Mylvaganam, K, Bacskay, GB & Hush, NS (1999). Homogeneous conversion of methane to methanol. 1. Catalytic activation and functionalization of methane by *cis*-platin in sulfuric acid: a density functional study of the thermochemistry. *Journal of the American Chemical Society* 121, 4633–4639.

Reimers, JR, Hall, LE, Crossley, MJ & Hush, NS (1999). Rigid fused oligoporphyrins as potential versatile molecular wires. 2. B3LYP and SCF calculated geometric and electronic properties of 98 oligoporphyrin and related molecules. *The Journal of Physical Chemistry A* 103, 4385–4397.

Reimers, JR & Hush, NS (1999). Electron and energy transfer through bridged systems. 9. Toward *a priori* evaluation of the intermetallic coupling in bis-metal complexes. *The Journal of Physical Chemistry A* 103, 3066–3072.

Reimers, JR & Hush, NS (1999). Vibrational Stark spectroscopy 3. Accurate benchmark *ab initio* and density functional calculations for CO and CN⁻. *The Journal of Physical Chemistry A* 103, 10580–10587.

2000

Hall, LE, Reimers, JR, Hush, NS & Silverbrook, K (2000). Formalism, analytical model, and *a priori* Green's-function-based calculations of the current–voltage characteristics of molecular wires. *The Journal of Chemical Physics* 112, 1510–1521.

Hush, NS & Reimers, JR (2000). Solvent effects on the electronic spectra of transition metal complexes. *Chemical Reviews* 100, 775–786.

Mylvaganam, K, Bacskay, GB & Hush, NS (2000). Homogeneous conversion of methane to methanol. 2. Catalytic activation of methane by *cis*- and *trans*-platin: a density functional study of the Shilov type reaction. *Journal of the American Chemical Society* 122, 2041–2052.

Reimers, JR, Hall, LE & Hush, NS (2000). Tautomerization of nucleobase model compounds: the 4-pyridinol and 4(1*H*)-pyridinone monomers and their dimers. *The Journal of Physical Chemistry A* 104, 5087–5092.

Reimers, JR, Hughes, JM & Hush, NS (2000). Modeling the bacterial photosynthetic reaction center 3: interpretation of effects of site-directed mutagenesis on the special-pair midpoint potential. *Biochemistry* 39, 16185–16189.

Reimers, JR, Hutter, MC, Hughes, JM & Hush, NS (2000). Nature of the special-pair radical cation in bacterial photosynthesis. *International Journal of Quantum Chemistry* 80, 1224–1243.

2001

Hughes, JM, Hutter, MC, Reimers, JR & Hush, NS (2001). Modeling the bacterial photosynthetic reaction center. 4. The structural, electrochemical, and hydrogen-bonding properties of 22 mutants of *Rhodobacter sphaeroides*. *Journal of the American Chemical Society* 123, 8550–8563.

Mylvaganam, K, Bacskay, GB & Hush, NS (2001). Protonation-induced paramagnetism. Structures and stabilities of six- and seven-coordinate complexes of Os(II) in singlet and triplet states: a density functional study. *Journal of the American Chemical Society* 123, 5495–5506.

Reimers, JR & Hush, NS (2001). The need for quantum-mechanical treatment of capacitance and related properties of nanoelectrodes. *The Journal of Physical Chemistry B* 105, 8979–8988.

2002

Bilić, A, Reimers, JR & Hush, NS (2002). Adsorption of pyridine on the gold(111) surface: implications for "alligator clips" for molecular wires. *The Journal of Physical Chemistry B* 106, 6740–6747.

Bilić, A, Reimers, JR, Hush, NS & Hafner, J (2002). Adsorption of ammonia on the gold (111) surface. *The Journal of Chemical Physics* 116, 8981–8987.

Lambropoulos, NA, Reimers, JR & Hush, NS (2002). Binding to gold(0): accurate computational methods with application to AuNH₃. *The Journal of Chemical Physics* 116, 10277–10286.

Reimers, JR, Hush, NS & Crossley, MJ (2002). Inter-porphyrin coupling: how strong should it be for molecular electronics applications? *Journal of Porphyrins and Phthalocyanines* 6, 795–805.

Reimers, JR, Shapley, WA, Lambropoulos, N & Hush, NS (2002). An atomistic approach to conduction between nanoelectrodes through a single molecule. *Annals of the New York Academy of Sciences* 960, 100–130.

Sendt, K, Johnston, LA, Hough, WA, Crossley, MJ, Hush, NS & Reimers, JR (2002). Switchable electronic coupling in model oligoporphyrin molecular wires examined

through the measurement and assignment of electronic absorption spectra. *Journal of the American Chemical Society* 124, 9299–9309.

Shapley, WA, Reimers, JR & Hush, NS (2002). INDO/S parameters for gold. *International Journal of Quantum Chemistry* 90, 424–438.

2003

Bilić, A, Reimers, JR & Hush, NS (2003). Modeling the adsorption of norbornadiene on the Si(001) surface: the predominance of non-[2+2]-cycloaddition products. *The Journal of Chemical Physics* 119, 1115–1126.

Binstead, RA, Reimers, JR & Hush, NS (2003). Inter-porphyrin coupling: rotation-modulation of inter-ring coupling in a μ -oxo-silicon phthalocyanine dimer. *Chemical Physics Letters* 378, 654–659.

Hush, NS (2003). An overview of the first half-century of molecular electronics. *Annals of the New York Academy of Sciences* 1006, 1–20.

Hush, NS (2003). Molecular electronics: cool computing. *Nature Materials* 2, 134–135.

Reimers, JR, Cai, Z-L, Bilić, A & Hush, NS (2003). The appropriateness of density-functional theory for the calculation of molecular electronics properties. *Annals of the New York Academy of Sciences* 1006, 235–251.

Reimers, JR & Hush, NS (2003). Modeling the bacterial photosynthetic reaction center. VII. Full simulation of the intervalence hole-transfer absorption spectrum of the special-pair radical cation. *The Journal of Chemical Physics* 119, 3262–3277.

Reimers, JR, Shapley, WA & Hush, NS (2003). Modelling the bacterial photosynthetic reaction center. V. Assignment of the electronic transition observed at 2200 cm^{-1} in the special-pair radical-cation as a second-highest occupied molecular orbital to highest occupied molecular orbital transition. *The Journal of Chemical Physics* 119, 3240–3248.

Reimers, JR, Shapley, WA, Rendell, AP & Hush, NS (2003). Modelling the bacterial photosynthetic reaction center. VI. Use of density-functional theory to determine the nature of the vibronic coupling between the four lowest-energy electronic states of the special-pair radical cation. *The Journal of Chemical Physics* 119, 3249–3261.

2004

Bilić, A, Reimers, JR, Hofer, WA & Hush, NS (2004). Adsorption sites of maleic anhydride on Si(100) revisited: inter- versus intra-row attachment. *Chemical Physics Letters* 385, 341–344.

- Bilić, A, Reimers, JR & Hush, NS (2004). Dissociated water on Si(100): relation between STM topograph and actual geometry. *Surface Review and Letters* 11, 185–190.
- Lambropoulos, NA, Reimers, JR & Hush, NS (2004). Flanged nanotube-electrode junctions. *Nanotechnology* 15, 1226.
- Reimers, JR, Bilić, A, Cai, Z-L, Dahlbom, M, Lambropoulos, NA, Solomon, GC, Crossley, MJ & Hush, NS (2004). Molecular electronics: from basic chemical principles to photosynthesis to steady-state through-molecule conductivity to computer architectures. *Australian Journal of Chemistry* 57, 1133–1138.
- Reimers, JR & Hush, NS (2004). A unified description of the electrochemical, charge distribution, and spectroscopic properties of the special-pair radical cation in bacterial photosynthesis. *Journal of the American Chemical Society* 126, 4132–4144.
- Reimers, JR & Hush, NS (2004). Hamiltonian operators including both symmetric and antisymmetric vibrational modes for vibronic coupling and intervalence charge-transfer applications. *Chemical Physics* 299, 79–82.
- Solomon, GC, Reimers, JR & Hush, NS (2004). Single molecule conductivity: the role of junction-orbital degeneracy in the artificially high currents predicted by *ab initio* approaches. *The Journal of Chemical Physics* 121, 6615–6627.
- Wang, B, Zheng, X, Michl, J, Foley, ET, Hersam, MC, Bilić, A, Crossley, MJ, Reimers, JR & Hush, NS (2004). An azanorbornadiene anchor for molecular-level construction on silicon(100). *Nanotechnology* 15, 324.

2005

- Bilić, A, Reimers, JR & Hush, NS (2005). The structure, energetics, and nature of the chemical bonding of phenylthiol adsorbed on the Au(111) surface: implications for density-functional calculations of molecular-electronic conduction. *The Journal of Chemical Physics* 122, 094708.
- Hush, NS, Schamberger, J & Bacskey, GB (2005). A quantum chemical computational study of the relative stabilities of *cis*- and *trans*-platinum dichloride in aqueous solution. *Coordination Chemistry Reviews* 249, 299–311.
- Reimers, JR, Cai, Z-L & Hush, NS (2005). *A priori* evaluation of the solvent contribution to the reorganization energy accompanying intramolecular electron transfer: predicting the nature of the Creutz–Taube ion. *Chemical Physics* 319, 39–51.
- Reimers, JR & Hush, NS (2005). The nature of the special-pair radical cation produced by primary charge separation during photosynthesis. Pages 109–126 in *Artificial*

Photosynthesis: from basic biology to industrial application, ed. by AF Collings & C Critchley. Wiley-VCH, Weinheim.

Solomon, GC, Reimers, JR & Hush, NS (2005). Overcoming computational uncertainties to reveal chemical sensitivity in single molecule conduction calculations. *The Journal of Chemical Physics* 122, 224502.

Zhang, J, Bilić, A, Reimers, JR, Hush, NS & Ulstrup, J (2005). Coexistence of multiple conformations in cysteamine monolayers on Au(111). *The Journal of Physical Chemistry B* 109, 15355–15367.

2006

Bilić, A, Reimers, JR & Hush, NS (2006). Functionalization of semiconductor surfaces by organic layers: concerted cycloaddition versus stepwise free-radical reaction mechanisms. Pages 333–360 in *Properties of Single Organic Molecules on Crystal Surfaces*, ed. by P Grütter, W Hofer & F Rosei. World Scientific Publishing Co., Singapore.

Bilić, A, Reimers, JR, Hush, NS, Hoft, RC & Ford, MJ (2006). Adsorption of benzene on copper, silver, and gold surfaces. *Journal of Chemical Theory and Computation* 2, 1093–1105.

Canfield, P, Dahlbom, MG, Hush, NS & Reimers, JR (2006). Density-functional geometry optimization of the 150 000-atom photosystem-I trimer. *The Journal of Chemical Physics* 124, 024301.

Gagliardi, A, Solomon, GC, Pecchia, A, Di Carlo, A, Frauenheim, T, Reimers, JR & Hush, NS (2006). Simulations of inelastic tunnelling in molecular bridges. Pages 183–186 in *Nonequilibrium Carrier Dynamics in Semiconductors*, ed. by M Saraniti & U Ravaioli. Springer Proceedings in Physics, volume 110. Springer, Berlin.

Kanchanawong, P, Dahlbom, MG, Treynor, TP, Reimers, JR, Hush, NS & Boxer, SG (2006). Charge delocalization in the special-pair radical cation of mutant reaction centers of *Rhodobacter sphaeroides* from Stark spectra and nonadiabatic spectral simulations. *The Journal of Physical Chemistry B* 110, 18688–18702.

Solomon, GC, Gagliardi, A, Pecchia, A, Frauenheim, T, Di Carlo, A, Reimers, JR & Hush, NS (2006). Understanding the inelastic electron-tunneling spectra of alkanedithiols on gold. *The Journal of Chemical Physics* 124, 094704.

Solomon, GC, Gagliardi, A, Pecchia, A, Frauenheim, T, Di Carlo, A, Reimers, JR & Hush, NS (2006). The symmetry of single-molecule conduction. *The Journal of Chemical Physics* 125, 184702.

Solomon, GC, Gagliardi, A, Pecchia, A, Frauenheim, T, Di Carlo, A, Reimers, JR & Hush, NS (2006). Molecular origins of conduction channels observed in shot-noise measurements. *Nano Letters* 6, 2431–2437.

2007

- Dastoor, PC, McNeill, CR, Frohne, H, Foster, CJ, Dean, B, Fell, CJ, Belcher, WJ, Campbell, WM, Officer, DL, Blake, IM, Thordarson, P, Crossley, MJ, Hush, NS & Reimers, JR (2007). Understanding and improving solid-state polymer/C₆₀-fullerene bulk-heterojunction solar cells using ternary porphyrin blends. *The Journal of Physical Chemistry C* 111, 15415–15426.
- Gagliardi, A, Solomon, GC, Pecchia, A, Frauenheim, , Di Carlo, A, Hush, NS & Reimers, JR (2007). *A priori* method for propensity rules for inelastic electron tunneling spectroscopy of single-molecule conduction. *Physical Review B* 75, 174306.
- Leiger, K, Freiberg, A, Dahlbom, MG, Hush, NS & Reimers, JR (2007). Pressure-induced spectral changes for the special-pair radical cation of the bacterial photosynthetic reaction center. *The Journal of Chemical Physics* 126, 215102.
- Reimers, JR, Solomon, GC, Gagliardi, A, Bilić, A, Hush, NS, Frauenheim, T, Di Carlo, A & Pecchia, A. (2007). The Green's function density functional tight-binding (gDFTB) method for molecular electronic conduction. *The Journal of Physical Chemistry A* 111, 5692–5702.
- Ren, W, Reimers, JR, Hush, NS, Zhu, Y, Wang, J & Guo, H (2007). Models for the structure and electronic transmission of carbon nanotubes covalently linked by a molecular bridge via amide couplings. *The Journal of Physical Chemistry C* 111, 3700–3704.
- Wang, Y, de Gironcoli, S, Hush, NS & Reimers, JR (2007). Successful *a priori* modeling of CO adsorption on Pt(111) using periodic hybrid density functional theory. *Journal of the American Chemical Society* 129, 10402–10407.
- Wang, Y, Hush, NS & Reimers, JR (2007). Formation of the gold-methanethiyl self-assembled monolayers. *Journal of the American Chemical Society* 129, 14532–14533.
- Wang, Y, Hush, NS & Reimers, JR (2007). Simulation of the Au(111) - ($22 \times \sqrt{3}$) surface reconstruction. *Physical Review B* 75, 233416.
- Wang, Y, Hush, NS & Reimers, JR (2007). Understanding the chemisorption of 2-methyl-2-propanethiol on Au(111). *Journal of Physical Chemistry C* 111, 10878–10885.
- Yin, S, Dahlbom, MG, Canfield, PJ, Hush, NS, Kobayashi, R & Reimers, JR (2007). Assignment of the Q_y absorption spectrum of photosystem-I from *Thermosynechococcus elongatus* based on CAM-B3LYP calculations at the PW91-optimized protein structure. *The Journal of Physical Chemistry B* 111, 9923–9930.

2008

- Day, P, Hush, NS & Clark, RJH (2008). Mixed valence: origins and developments. *Philosophical Transactions of the Royal Society, A* 366, 5–14.

Hush, NS (2008). Symmetry breaking, delocalization and dynamics in electron transfer systems. Pages 465–504 in *Physical Biology; from atoms to medicine*, ed. by AH Zewail. World Scientific Publishing Co., Singapore.

Reimers, JR, Wallace, BB & Hush, NS (2008). Towards a comprehensive model for the electronic and vibrational structure of the Creutz–Taube ion. *Philosophical Transactions of the Royal Society A* 366, 15–31.

2009

McKemmish, LK, Reimers, JR, McKenzie, RH, Mark, AE & Hush, NS (2009). Penrose-Hameroff orchestrated objective-reduction proposal for human consciousness is not biologically feasible. *Physical Review E* 80, 021912.

Reimers, JR, McKemmish, LK, McKenzie, RH, Mark, AE & Hush, NS (2009). Weak, strong, and coherent regimes of Fröhlich condensation and their applications to terahertz medicine and quantum consciousness. *Proceedings of the National Academy of Sciences of the USA* 106, 4219–4224.

Wang, Y, Chi, Q, Hush, NS, Reimers, JR, Zhang, J & Ulstrup, J (2009). Scanning tunneling microscopic observation of adatom-mediated motifs on gold–thiol self-assembled monolayers at high coverage. *The Journal of Physical Chemistry C* 113, 19601–19608.

2010

Wohlthat, S, Reimers, JR & Hush, NS (2010). Accurate and computationally efficient third-nearest-neighbor tight-binding model for large graphene fragments. *Physical Review B* 81, 195125.

2011

Chin, Y, Panduwinata, D, Santic, M, Sum, T-J, Hush, NS, Crossley, MJ & Reimers, JR (2011). Atomic-resolution kinked structure of an alkylporphyrin on highly ordered pyrolytic graphite. *The Journal of Physical Chemistry Letters* 2, 62–66.

McKemmish, LK, McKenzie, RH, Hush, NS & Reimers, JR (2011). Quantum entanglement between electronic and vibrational degrees of freedom in molecules. *The Journal of Chemical Physics* 135, 244110.

Wang, Y, Chi, Q, Hush, NS, Reimers, JR, Zhang, J & Ulstrup, J (2011). Gold mining by alkanethiol radicals: vacancies and pits in the self-assembled monolayers of 1-propanethiol and 1-butanethiol on Au(111). *The Journal of Physical Chemistry C* 115, 10630–10639.

Wang, Y, Chi, Q, Zhang, J, Hush, NS, Reimers, JR & Ulstrup, J (2011). Chain-branching control of the atomic structure of alkanethiol-based gold–sulfur interfaces. *Journal of the American Chemical Society* 133, 14856–14859.

Wohlthat, S, Solomon, GC, Hush, NS & Reimers, JR (2011). Interference-induced electron- and hole-conduction asymmetry. *Theoretical Chemistry Accounts* 130, 815–828.

2012

McKemmish, LK, Kedziora, DJ, White, GR, Hush, NS & Reimers, JR (2012). Frequency-based quantum computers from a chemist's perspective. *Australian Journal of Chemistry* 65, 512–519.

2013

Lambropoulos, NA, Reimers, JR, Crossley, MJ, Hush, NS & Silverbrook, K (2013). A multiscale simulation technique for molecular electronics: design of a directed self-assembled molecular *n*-bit shift register memory device. *Nanotechnology* 24, 505202.

2014

Kuchel, PW, Naumann, C, Chapman, BE, Shishmarev, D, Håkansson, P, Bacskey, G & Hush, NS (2014). NMR resonance splitting of urea in stretched hydrogels: proton exchange and $^1\text{H}/^2\text{H}$ isotopologues. *Journal of Magnetic Resonance* 247, 72–80.

Reimers, JR, McKemmish, LK, McKenzie, RH, Mark, AE & Hush, NS (2014). The revised Penrose–Hameroff orchestrated objective-reduction proposal for human consciousness is not scientifically justified Comment on “Consciousness in the universe: A review of the ‘Orch OR’ theory” by Hameroff and Penrose. *Physics of Life Reviews* 11, 101–103.

Yan, J, Ouyang, R, Jensen, PS, Ascic, E, Tanner, D, Mao, B, Zhang, J, Tang, C, Hush, NS, Ulstrup, J & Reimers, JR (2014). Controlling the stereochemistry and regularity of butanethiol self-assembled monolayers on Au(111). *Journal of the American Chemical Society* 136, 17087–17094.

2015

McKemmish, LK, McKenzie, RH, Hush, NS & Reimers, JR (2015). Electron–vibration entanglement in the Born–Oppenheimer description of chemical reactions and spectroscopy. *Physical Chemistry Chemical Physics* 17, 24666–24682.

Ouyang, R, Yan, J, Jensen, PS, Ascic, E, Gan, S, Tanner, D, Mao, B, Niu, L, Zhang, J, Tang, C, Hush, NS, Reimers, JR & Ulstrup, J (2015). Intermixed adatom and surface-bound adsorbates in regular self-assembled monolayers of racemic 2-butanethiol on Au(111). *ChemPhysChem* 16, 928–932.

Reimers, JR, McKemmish, LK, McKenzie, RH & Hush, NS (2015). A unified diabatic description for electron transfer reactions, isomerization reactions, proton transfer reactions, and aromaticity. *Physical Chemistry Chemical Physics* 17, 24598–24617.

Reimers, JR, McKemmish, LK, McKenzie, RH & Hush, NS (2015). Bond angle variations in XH_3 [X = N, P, As, Sb, Bi]: the critical role of Rydberg orbitals exposed using a diabatic state model. *Physical Chemistry Chemical Physics* 17, 24618–24640.

Reimers, JR, McKemmish, LK, McKenzie, RH & Hush, NS (2015). Non-adiabatic effects in thermochemistry, spectroscopy and kinetics: the general importance of all three Born–Oppenheimer breakdown corrections. *Physical Chemistry Chemical Physics* 17, 24641–24665.

Reimers, JR, Panduwinata, D, Visser, J, Chin, Y, Tang, C, Goerigk, L, Ford, MJ, Sintic, M, Sum, T-J, Coenen, MJJ, Hendriksen, BLM, Elemans, JAAW, Hush, NS & Crossley, MJ (2015). A priori calculations of the free energy of formation from solution of polymorphic self-assembled monolayers. *Proceedings of the National Academy of Sciences of the USA* 112, E6101–6110.

2016

Chi, Q, Halder, A, Hush, NS, Reimers, JR, Ulstrup, J & Zhang, J (2016). En ny historie om guld og svovl - guld - svovlbindingen i thiolers adsorption på guldnanopartikler og plane guldoverflader. *Dansk Kemi* 97, 20–23.

Reimers, JR, Ford, MJ, Halder, A, Ulstrup, J & Hush, NS (2016). Gold surfaces and nanoparticles are protected by Au(0)–thiyl species and are destroyed when Au(1)–thiolates form. *Proceedings of the National Academy of Sciences of the USA* 113, E1424–1433.

Reimers, JR, Panduwinata, D, Visser, J, Chin, Y, Tang, C, Goerigk, L, Ford, MJ, Baker, M, Sum, T-J, Coenen, MJJ, Hendriksen, BLM, Elemans, JAAW, Hush, NS & Crossley, MJ (2016). From chaos to order: chain-length dependence of the free energy of formation of meso-tetraalkylporphyrin self-assembled monolayer polymorphs. *The Journal of Physical Chemistry C* 120, 1739–1748.

2017

Chi, Q, Ford, MJ, Halder, A, Hush, NS, Reimers, JR & Ulstrup, J (2017). Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: what, how and why. *Current Opinion in Electrochemistry* 1, 7–15.

Ford, MJ, Hush, NS, Marcuccio, S, Reimers, JR, Ulstrup, J & Zhang, J (2017). The Au-S bond in biomolecular adsorption and electrochemical electron transfer. Abstract, *2nd Gerischer-Kolb Symposium*, Günzburg/Donau, Germany.

Hush, NS (2017). A glimpse of the evolution of adiabaticity. Pages 141–151 in *Personal and Scientific Reminiscences: tributes to Ahmed Zewail*, ed. by M Chergui, RA Marcus, JM Thomas & D Zhong. World Scientific Publishing Co., Singapore.

Hush, NS & Radom, L (2017). David Parker Craig 1919–2015. *Historical Records of Australian Science* 28, 159–170.

- Hush, NS & Radom, L (2017). David Parker Craig AO FAA. 23 December 1919–1 July 2015. *Biographical Memoirs of Fellows of the Royal Society* 64, 107–129.
- Reimers, JR, Ford, MJ, Marcuccio, SM, Ulstrup, J & Hush, NS (2017). Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles. *Nature Reviews Chemistry* 1, article 0017. Erratum published March 2017 in article 0034.
- Reimers, JR & Hush, NS (2017). Relating transition-state spectroscopy to standard chemical spectroscopic processes. *Chemical Physics Letters* 683, 467–477.
- Reimers, JR & Hush, NS (2017). The critical role of the transition-state cusp diameter in understanding adiabatic and non-adiabatic electron transfer. *Russian Journal of Electrochemistry* 53, 1042–1053.
- Reimers, JR, McKemmish, LK, McKenzie, RH & Hush, NS (2017). Diabatic models with transferrable parameters for generalized chemical reactions. *Journal of Physics: Conference Series* 833, 012014.

2019

- Yang, L, Reimers, JR, Kobayashi, R & Hush, NS (2019). Competition between charge migration and charge transfer induced by nuclear motion following core ionization: model systems and application to Li_2^+ . *The Journal of Chemical Physics* 151, 124108.

DAY 4 | Thursday, July 4th 2024 HUSH SYMPOSIUM

Lecture Room 1070, University of Sydney Business School

Session 1 Chair: Alison Rodger, ANU

9:00 – 9:05	Welcome and Acknowledgement of Country
9:05 – 9:20	Jeff Reimers , University of Technology, Sydney & Shanghai University <i>Noel Hush career overview, eulogy and tributes</i>
9:20 – 9:50	Plenary Talk: Steve Boxer , Stanford University <i>Continuing impact of Noel Hush on physical science: A personal view</i>
9:50 – 10:10	H1: Jens Ulstrup , Technical University of Denmark <i>New stories about gold and sulfur – 30 years+ with Noel Hush and Jeffrey Reimers</i>
10:10 – 10:30	H2: Philip Kuchel , The University of Sydney <i>My links to Noel Hush</i>
10:30– 10:55	MORNING TEA

Session 2 Chair: Tim Schmidt, UNSW

10:55 – 11:10	H3: Ken Ghiggino , The University of Melbourne <i>Some personal perspectives on photoinduced electron transfer in linked molecular systems</i>
11:10 – 11:30	H4: Laura McKemmish , UNSW <i>Noel's legacy: Treating students as respected colleagues</i>
11:30 – 11:35	H5: Mick Collins , ANU <i>The early years of theoretical chemistry at Sydney</i>
11:35 – 11:55	H6: Jack Evans , The University of Adelaide <i>Historic and modern simulation methods to examine soft pores and amorphous solids</i>
11:55 – 12:15	H7: Jun Zeng , Qubist Molecular Design and MedChemSoft Solutions <i>From quantum chemistry to drug discovery: Development of billion-dollar drug Ojjaara</i>
12:15 – 12:35	H8: Murad Tayebjee , UNSW <i>Delving into the intricate world of singlet fission</i>
12:35 – 13:25	LUNCH

Session 3 Chair: Debra Bernhardt, The University of Queensland

13:25 – 13:35	H9: Julia Hush
13:35 – 13:55	H10: Peter Taylor , Tianjin University <i>The view from the left, the view from the right...</i>
13:55 – 14:00	H11: Shiwei Yin , Shaanxi Normal University <i>My Electron transfer "dream"</i>
14:00 – 14:05	H12: Damon Ridley , The University of Sydney <i>Interview</i>
14:05 – 14:25	H13: Brian Yates , University of Tasmania <i>Noel Hush – A powerful catalyst for physical chemistry</i>
14:25 – 14:45	H14: David Wilson , La Trobe University <i>Theoretical insights of beryllium chemistry</i>
14:45 – 15:05	H15: Yun Wang , Griffith University <i>Operando simulation for electrocatalyst design</i>
15:05 – 15:30	AFTERNOON TEA

Session 4 Chair: Ivan Kassal, The University of Sydney	
15:30 – 15:50	H16: Robin Purchase, ANU <i>Identification of the chromophores in prussian blue</i>
15:50 – 16:05	H17: Muhammad Nadeem, The University of Queensland <i>Complex Relaxation of Trapped Spin-States in Spin Crossover Materials</i>
16:05 – 16:25	H18: John Dyke, University of Southampton <i>Examples from my research which show guidance, training and advice I received from Noel Hush</i>
16:25 – 16:45	H19: Bob Gilbert <i>Closing remarks and Finale</i>
16:45 – 17:00	Change of venue
Hush Symposium Public Lecture Lecture Theatre 1130, University of Sydney Business School	
Chair Palli Thordarson, UNSW, President, Royal Australian Chemical Institute	
17:00 – 18:00	Public Lecture: Cathy Foley, AO PSM FAA FTSE Australian Chief Scientist and Industry Innovation and Science Australia board deputy chair