THE UNIVERSITY OF SYDNEY

Hush Lecture 2024

Professor Benjamin J. Schwartz

Friday 13th September 2024

New Law Lecture Theatre 104

About the Hush Lectureship

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.

Plinth and plaque outside of the School of Chemistry built in memory of Professor Noel Hush

Professor Noel Hush

Noel Hush was born and educated in Sydney, receiving his MSc from The University of Sydney in 1948. He took up a Lectureship at Manchester in 1950, working on the theory of diffusion-reaction kinetics of electrode processes and on energetics of oxidation–reduction processes in solution. Hush then moved in 1954 to the Bristol University Chemistry Department. In 1971 he was invited to return to The University of Sydney as Foundation Professor of Theoretical Chemistry where he set up the Department of Theoretical Chemistry at the University of Sydney – the first such department in Australia.

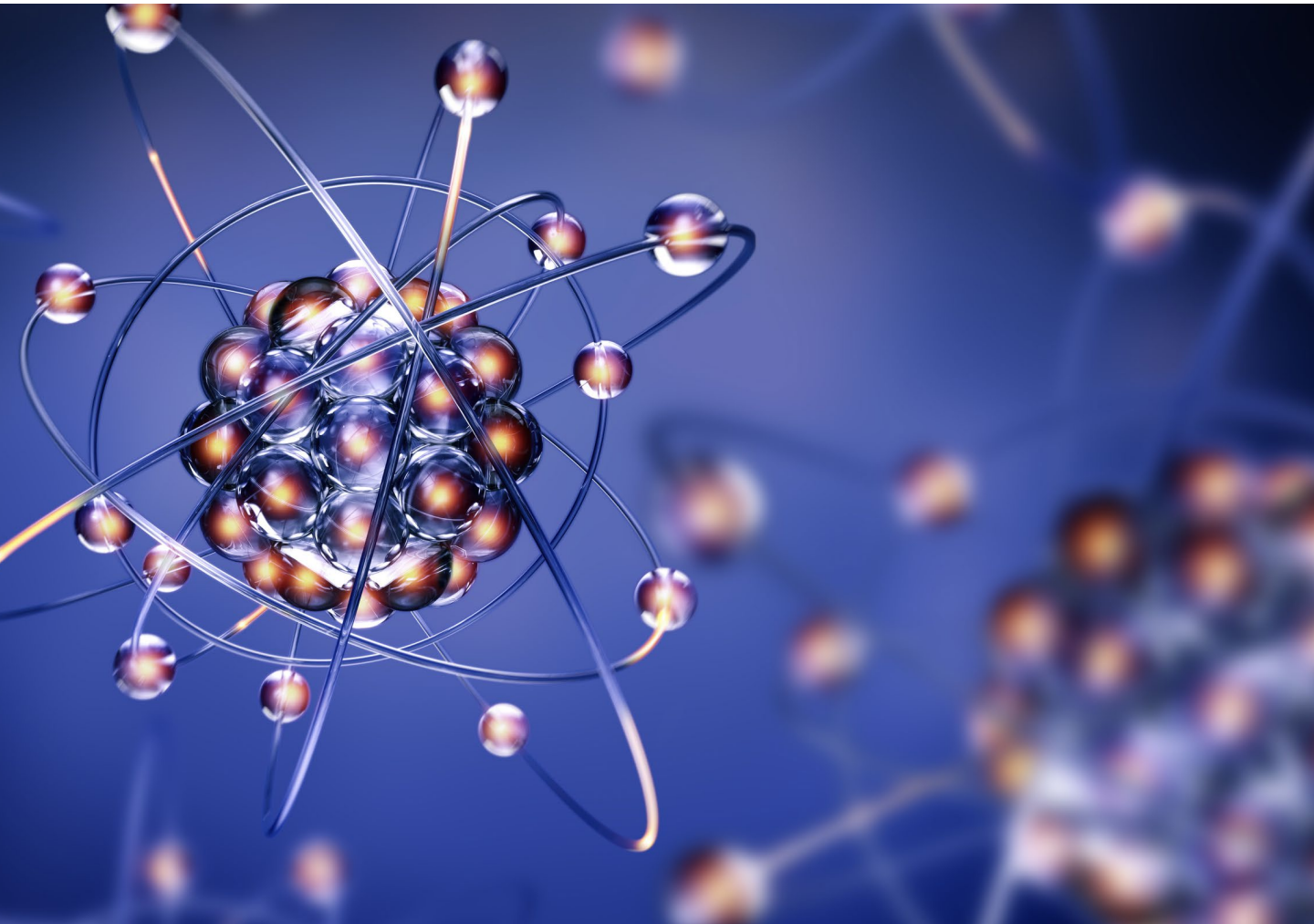
Hush was a theoretical and computational chemist whose contributions have significantly influenced diverse fields, including corrosion, photosynthesis, solar energy, and molecular electronics. Most notably, he is recognised for the development of the chemical electron transfer model – a model now universally acknowledged as the mechanism by which chemical reactions occur.

Hush was elected as fellow of the Royal Australian Chemical Institute (FRACI), Australian Academy of Science (FAA), the Royal Society (FRS), American Academy of Arts and Sciences, and the Royal Society of New South Wales (FRNS). He was also awarded several prestigious awards including the Order of Australia (AO) in 1993.

Noel Hush passed away in 2019 at the age of 94. He is remembered for his invaluable contributions to the field of chemistry, and a research career spanning eight decades.

Previous Lecturers

2009	Abraham Nitzan Tel Aviv University
2014	David Clary Oxford University
2015	Steven Boxer Stanford University



Professor Benjamin J. Schwartz

Department of Chemistry and Biochemistry, UCLA

Benjamin J. Schwartz received his Bachelor's degree in Physics and Chemistry from the University of Michigan in 1986, and his Ph.D. in Experimental Physical Chemistry from UC Berkeley in 1992, working under Prof. Charles Harris. After postdoctoral work in theoretical physical chemistry at the University of Texas, Austin (1993-5 with Prof. Peter Rossky) and in the spectroscopy and device physics of semiconducting polymers at UC Santa Barbara (1995-6, with 2000 Nobel Laureate Alan Heeger), he joined UCLA in 1997. He was promoted to Associate Professor with tenure in 2002, Full Professor in 2004, and Distinguished Professor in 2022. He has given over 200 invited lectures, published over 200 papers in peer-reviewed journals, and holds 2 U.S. patents with an additional patent pending. Prof. Schwartz has received Teacher-Scholar awards from both the Dreyfus Foundation and the Research Corporation, and he is a Sloan Foundation Fellow. His leadership experience includes serving for 8 years as Vice-Chair of the Department of Chemistry and Biochemistry. His teaching has been recognized by the department's Hanson-Dow award and UCLA's campus-wide Distinguished Teaching Award. Prof. Schwartz served as Senior Editor for the Journal of Physical Chemistry for 14 years, and in 2019 started as Senior Editor for the Journal of Physical Chemistry Letters. His current research interests include quantum non-adiabatic processes in condensed phases studied from both theoretical and ultrafast spectroscopic points of view, solvated electrons, and studies of the fundamental processes, spectroscopy, and device physics underlying the operation of conjugated polymer-based optoelectronic devices.

The Role of the Solvent in Chemical Identity, Chemical Reactivity and Quantum Decoherence

For simple solution-phase chemical reactions, such as the photodissociation of a diatomic molecule, is it appropriate to assume that the potentials energy surfaces of the molecule are the same in solution as in the gas phase? If not, what modifications need to be made because of the solute-solvent interactions to understand the electronic structure and reactivity of molecules in solution? When the solvent determines the outcome of a chemical reaction, how does it induce quantum decoherence, and can decoherence be controlled? Here, we work to answer these questions using theoretical methods, focusing on simple solutes such as Na2, Na2+ and NaK+. We find that the interactions with the solvent not only control the bond dynamics of the solute, but that the solvent can actually become part of the chemical identity of the solute. This can cause the excited-state dynamics to no longer follow the simple photodissociation observed in the gas phase; instead, the excited-state motion involves isomerization of the local solvent molecules and requires a two-dimensional potential energy surface to describe. The solvent-induced change in chemical identity can also change the products of simple dissociation reactions relative to what is observed in the gas phase. We also investigate how solvents cause quantum decoherence, for example, determining whether Na2+ dissociation leads to Na + Na+ or Na+ + Na products. We use machine learning to focus on isolating the subset of solvent motions that cause the decoherence that chooses the products, which involve asymmetric collisions on the two atomic fragments once they are separated enough to no longer behave like a single molecule.