

## J.K.N. JONES

John Kenyon Netherton Jones, Ph.D. Birmingham University. Assistant lecturer and then lecturer at Bristol University 1936-1944, he was engaged in munitions research and training during the Second World War. He resigned at the end of the war with the rank of captain, and returned to academic work as senior lecturer at Manchester University 1945-1948 and then as reader in chemistry at Bristol University 1948-1953. He came to Queen's in 1953 as Chown Research Professor of Chemistry, a position he held until his death in 1977.

Professor Jones' outstanding achievements in carbohydrate chemistry were recognized by his election as Fellow of the Royal Society of London in 1957 and of the Royal Society of Canada in 1959. The Division of Carbohydrate Chemistry of the American Chemical Society presented him with the Claude S. Hudson Award in 1969, and in 1975 he received the Anselme Payen Award from the Cellulose, Paper and Textile Division. In March 1975 he was awarded the third Sir Norman Haworth Memorial Medal of The Chemical Society (London).

Professor Jones was, at all times, an educator of the highest rank and an inspiration to a large number of graduate students, from whom he evoked, as a result of his enthusiasm, sincerity, and gentle character, tremendous respect and affection. All of his students, former research associates, colleagues, and friends will long remember this truly fine and outstanding gentleman.

The J.K.N. Jones Visitorship was established in memory of Professor Jones, and is funded by the income from the bequests made in his name by his friends, colleagues and former students.

## PREVIOUS JONES LECTURERS

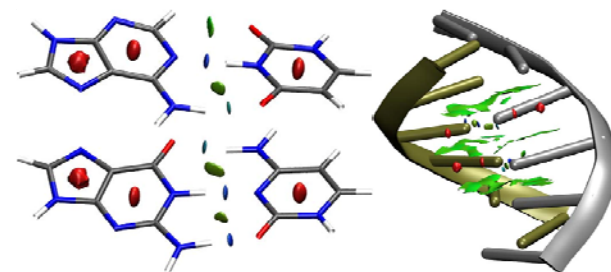
- 2013 • *D. Milstein*
- 2012 • *J.F. Stoddard*
- 2011 • *J.A. Caruso*
- 2010 • *T. Marks*
- 2010 • *G. van Koten*
- 2009 • *P.B. Corkum*
- 2008 • *M. Gruebele*
- 2005 • *W. Klemperer*
- 2001 • *G. Ozin*
- 1997 • *M.S. Brookhart*
- 1993 • *B.O. Fraser-Reid*
- 1990 • *S. Hanessian*
- 1982 • *R. U. Lemieux*



### Department of Chemistry Queen's University

is honoured to host the  
2014 Jones Lecturer:

Prof. Weitao Yang  
Department of Chemistry,  
Duke University  
Durham, North Carolina



"The Wonders of Electron Density:  
From Half an Electron to  
Noncovalent Interactions of  
Biomolecular Complexes "

Friday, March 14, 2014  
11:30 am

Room 117, Chernoff Hall

## PROF. WEITAO YANG



### Professor Weitao Yang

Philip Handler Professor of Chemistry and Physics  
Department of Chemistry  
Duke University  
Durham, North Carolina

Weitao Yang was born in Chaozhou, China. He received his B.S. degree from Peking University and Ph.D. degree from the University of North Carolina at Chapel Hill. He is currently the Philip Handler Professor of Chemistry and Physics at Duke University. Yang's interests are in developing theory and applying it to complex problems in chemistry and biology.

Yang's major contributions have been in the development of theoretical and computational methods in electronic structure theory. His contributions have made electronic structure calculations much more efficient and accurate. Yang pioneered the development of the linear scaling divide-and-conquer method for electronic structure calculations of large systems. Development and applications of linear scaling methods have attracted much interest. Yang's 1991 Physical Review Letters paper marked the beginning of the linear scaling field.

Yang has contributed to the development of density-functionals that go beyond the local density-functional approximation. The Becke-Lee-Yang-Parr (B3LYP) density-functional, the combination of the Lee-Yang-Parr correlation functional with the Becke exchange functional, is the most widely used approximation in practical electronic structure calculations. His recent studies have revealed the origins of failure of common density functional approximations as the delocalization and state correlation error, through the perspectives of fractional charges and fractional spins. This further leads to the development of much improved approximations.

Yang has developed multiscale approaches combining methods of quantum chemistry and statistical mechanics to address the reaction mechanisms of solution and enzymatic catalysis.

Professor Yang has held visiting professorships from many institutions including the Japanese Society for Promotion of Science, Kyoto University, the University of Hong Kong, Tsinghua University, Peking University, South China Normal University and Vrije Universiteit Brussel.

#### Distinguished Lectures:

New Century Forum Distinguished Lecture, South China Normal University, "Free Energy and Mechanism of Chemical Reactions in Solution and in Enzymes", Guangzhou, China, December 9, 2009

Solvay Lecture, "The wonders of electron density: from half an electron to the noncovalent interactions of biomolecular complexes", the International Solvay Institutes, Brussels, November 9, 2010

Distinguished Lecture in Computational and Mathematical Biology, " Simulating chemical and redox processes in solution and in enzymes with multiscale approaches". University of California, Irvine, February 18, 2004

## SELECTED HONOURS & AWARDS

- Florida Award by the Florida Section of the American Chemical Society (2014)
- American Chemical Society National Award for Computers in Chemical and Pharmaceutical Research (2012)
- International Solvay Chair in Chemistry, International Solvay Institutes for Physics and Chemistry, Brussels, Belgium (2010)
- Humboldt Research Award for Senior U.S. Scientists (2006)
- Annual Medal of the International Academy of Quantum Molecular Science (1997)
- Sloan Fellowship (1993)
- Elected Fellow of American Association for the Advancement of Science and of the American Physical Society
- Elected member of the International Academy of Quantum Molecular Science (<http://www.IAQMS.org/>)
- Co-author (with Robert G. Parr) on one of the leading textbooks on density-functional theory
- 340 Plenary and Invited Talks
- Associate Editor, Theoretical Chemistry Accounts (2011-present)
- **Editorial Boards**
  - ◆ Journal of Chemical Physics (2012-present)
  - ◆ Chemical Physics (2012-present)
  - ◆ The International Journal of Quantum Chemistry (2002-present)
  - ◆ The Chinese Journal of Chemical Physics (2002-present)
  - ◆ The Acta Physico-Chimica Sinica (2000-present)
  - ◆ Theoretical Chemistry Accounts (1997-2012)