

Personal data

Name: Poul Jørgensen

Nationality: Danish

Date of birth: March 2, 1944, Silkeborg, Denmark

Education

•1975 Advanced doctoral degree in chemistry, Aarhus University

•1969 Cand. Scient. in chemistry, Aarhus University

Academic career

•2010 Advanced Research Professor of Chemistry, Aarhus University

•2001 Professor of Chemistry, Aarhus University

•1976 Associate Professor of Chemistry, Aarhus University

Visiting Professorships

•2005 University of Otago, Dunedin, New Zealand, 2 months

•1986 University of Minnesota, 2 months

•1982 Texas A&M University, 6 months

•1977, 1978, 1980, 1982, 1984, 1989, 1992, 1995, 2009 University of Utah, total period approx. 2 years

Project management

•2012–2017: Director of “The qLEAP Centre” funded (€ 1,73 million) by the European Research Council

•2006–2011: Director of “The Lundbeck Foundation Centre for Theoretical Chemistry” funded (€ 2,687,098) by the Lundbeck Foundation

•2004–2007: Director of “Centre for Theoretical Chemistry”, funded (€ 0.95 million) by the Danish Natural Science Research Council

Awards

•Awards for extraordinary scientific accomplishment by the International Conference of Computation Methods in Science and Engineering (ICCMSE). Crete, October 2006.

•Honoured by Thomson Scientific and the Danish Library Association as the most cited author in chemistry in Denmark, during the period 1990–2004. Copenhagen, May 2005.

•Rigmor and Carl Holst-Knudsens Videnskabspris, Aarhus University. Aarhus, May 1986

Books

•Molecular Electronic Structure Theory. Trygve Helgaker, Poul Jørgensen and Jeppe Olsen, Wiley, Chichester, 2000. ~ 1000 citations.

•Geometrical Derivatives of Energy Surfaces and Molecular Properties. Edited by Poul Jørgensen and Jack Simons, NATO ASI series, D. Reidel Publishing Company, Dordrecht, 1986. ~ 100 citations.

•Problems in Quantum Chemistry, Poul Jørgensen and Jens Oddershede, Addison Wesley, Reading, Massachusetts, 1982.

•Second Quantization Based Methods in Quantum Chemistry, Poul Jørgensen and Jack Simons, Academic Press, New York, 1981. ~ 400 citations.

Publications, presentations and bibliometric indicators

•More than 320 publications in peer reviewed international journals

•More than 65 invited talks at international conferences

•More than 21,000 citations

•h-index 73 (according to ISI Web of knowledge database)

•For 2007-2014: 39 publications in peer reviewed international journals

Important contributions

•Time-independent and time-dependent linear and non-linear response function theory

•Optimization theory for multi-configurational self-consistent field wave functions

•Coupled cluster theory: model hierarchies, molecular property evaluation, and linear-scaling and massively parallel algorithms

•Lagrangian technique for molecular property calculations

•Calculation of magnetic molecular properties using gauge invariant methods

•Showing and explaining the divergence of Møller–Plesset perturbation theory

•Benchmarking the accuracy of electronic structure models

•Basis set extrapolation for accurate calculations of energies

•Optimization theory for Hartree–Fock and Kohn Sham theory, including linear-scaling algorithms

•Localization of Hartree–Fock and Kohn Sham orbitals

Current funding

• CAAR partnership project with Oak Ridge National Laboratory (2015-2018). • U.S. Department of Energy: 128 million core hours (2014-2016) on supercomputer TITAN. Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award. •The European Research Council: € 1.73 million. Coupled Cluster Calculations on Large Molecular Systems. (2012 – 2017) •The Danish Council for Independent Research, Natural Sciences: € 442,092. Molecular Properties for Large Molecules Using the Divide-Expand-Consolidate Coupled Cluster Method (2011-2014)

Recent funding

•The Lundbeck Foundation: € 2,687,098. Quantum Mechanics for Large Molecular Systems (2006 – 2011).

•Danish Centre for Scientific Computing: € 288,403. Exploring Large Molecular Systems with Quantum Mechanics (funding for computer hardware). (2009 – 2011)

•Danish Centre for Scientific Computing: € 67,000. Quantum Mechanics for Large Molecular Systems (funding for computer hardware). (2008 – 2010)

- Danish Centre for Scientific Computing: € 187,000. Quantum Mechanics for Large Molecular Systems (funding for computer hardware). (2007 – 2009)

- The Danish Natural Science Research Council: € 0.95 million. Centre for Theoretical Chemistry (2004 – 2007)

Reviewing

- Has been reviewer for most journals in the field of physical chemistry and for the American, the Canadian, and most European natural science research councils e.g. as panel member for the German Research Foundation (2003 – 2009) in the high priority program "First-principles Methods for Many-Electron Systems in Chemistry and Physics"

Conference organizer

- 5 international conferences

Summer Schools

- Organized biannually since 1990 a two-week summer school (together with T. Helgaker, Oslo and J. Olsen, Aarhus) "Quantum Chemistry and Molecular Properties". Given about 16 lectures at each school.

- Been lecturer at five other summer schools.

Been supervisor for

- About 35 PhD students, among others:

Jeppe Olsen – currently professor at Aarhus University

Henrik Koch – currently professor at NTNU, Trondheim

Ove Christiansen – currently professor at Aarhus University

Sonia Coriani – currently associate professor at University of Trieste

- About 25 Post Docs, among others:

Trygve Helgaker – currently professor at University of Oslo

Christof Hättig – currently professor at University of Bochum

Hans Jørgen Aa. Jensen – currently associate professor at University of Southern Denmark

Berta Fernandez – currently professor at University of Santiago de Compostela