Curriculum vitae — Trygve Helgaker

Personal Information

Family name, First name: Helgaker, Trygve Ulf

Date of birth: *11.08.1953*

Nationality: Norwegian

Researcher unique identifier(s): orcid.org/0000-0002-5032-8392 Research ID: I-2062-2012

URL for personal web site:: http://www.mn.uio.no/kjemi/english/people/aca/helgaker

Education

1981–1986	*dr. philos:* theoretical chemistry, disputation date: 13.06.1986 Faculty of Mathematics and Natural Sciences, University of Oslo, Norway
1978–1980	*cand. scient.*: electron diffraction, Department of Chemistry, University of Oslo, Norway
1975–1978	*cand. mag.*: chemistry, mathematics, physics, and Russian, University of Oslo, Norway
1974–1975	University of Leningrad (Russian studies)
1972–1974	Norwegian Army Language School (Russian studies)

Current and Previous Positions

2017–	Director, Hylleraas Centre, Department of Chemistry, University of Oslo, Norway
2013–2017	Director, CTCC, Department of Chemistry, University of Oslo, Norway
1992–	Professor, Department of Chemistry, University of Oslo, Norway
1989–1992	Associate Professor, Department of Chemistry, University of Oslo, Norway
1987–1989	Researcher, Department of Chemistry, Aarhus University, Denmark
1986–1987	Researcher, Institute of Mathematics and Its Applications, University of Minnesota, USA
1985–1986	Associate Professor, Department of Chemistry, University of Oslo, Norway
1979–1979	Researcher, Department of Slavic Studies, University of Oslo, Norway

Mobility

2006 – 2007	Department of Chemistry, University of Durham, UK (12 months)
1999 – 2000	Department of Chemistry, University of Cambridge, UK (12 months)

Funding

2020 – 2023	*Magnetic Chemistry*, RCN 287950, **leader**, MNOK 11,009
2017 – 2022	*Hylleraas Centre of Excellence*, RCN 232395, **director**, MNOK 146,000
2017 – 2018	*Molecules in Extreme Environments*, Centre Adv. Study, Norway, **leader**, MNOK 3,500
2011 – 2016	*Advanced Grant*, ERC Grant No 267683, **leader**, EUR 2,100,000
2007 – 2017	*CTCC Centre of Excellence*, RCN 171185, **co-leader**, MNOK 93,863
2010 – 2013	*Molecules in Magnetic Fields*, RCN 197446, **leader**, MNOK 4,800
2006 – 2009	*SCF Methods for Periodic and Non-Periodic Systems,* RCN 171185, **leader**, MNOK 2,268
2004 – 2007	*NANOQUANT*, FP6 MRTN–CT-2003-506842, **partner**, EUR 1,781,000
2003 – 2007	*Strategic University Program in Quantum Chemistry*, RCN 154011, **partner**, MNOK 8,650
2003 – 2004	*Linear-Scaling Quantum-Chemical Methods for Large Systems*, RCN 155137, MNOK 1,362
2003 – 2006	Molecular Modelling in Nanotechnology, RCN 158538, **partner**, MNOK 8,291
2000 – 2003	MOLPROP, ETN, FP5 HPRN-2000-00013, **partner**, EUR 1,465,000 (EUR 175,572)
1999 – 2002	*Relativistic Corrections to Mol. Magnetic Properties*, RCN 132030, **leader**, MNOK 1,289

Supervision of Graduate Students and Research Fellows

1989 – 2021	(19/4) postdocs, (12/4) PhD students, (16/0) master students at the University of Oslo

Teaching Activities

1989 – 2013 undergraduate teaching in physical and theoretical chemistry (except for sabbaticals)

Institutional Responsibilities

2017 – 2020 Deputy Board Member, *Department of Chemistry*, University of Oslo
2014 – Advisory Board Member, *Centre for Integrative Neuroplasticity*, University of Oslo
2003 – 2012 Advisory Board Member, *Centre of Mathematics and Applications,* University of Oslo
2004 – 2006 Organiser of Department of Chemistry Seminar Series, University of Oslo
1989 – 1997 IT Committee Chair, Department of Chemistry, University of Oslo

Commissions of Trust

2020 – Group Leader Chemistry, Norwegian Academy of Science and Letters, Norway
2018 – Board Member, International Academy of Quantum Molecules Science
2015 – Hassel Lecture Committee Member, Norwegian Chemical Society, Norway
2015 – Academic Committee Member, Aker Scholarship, Norway
2013 – Editor, Molecular Physics, UK.
2011 – Advisory Board Member, WIREs Computational Molecular Science, UK
2010 – 2012 e-Infrastructure Scientific Opportunities Panel Member, Norway
2008 – 2018 Editorial Board Member, Chemical Physics Letters, UK
2007 – 2013 Advisory Board Member, Molecular Physics, UK
1998 – 2006 Editorial Board Member, Theoretical Chemistry Accounts, USA
1996 – Editorial Board Member, Inter. Journal of Quantum Chemistry, USA
1989 – opponent and member of 17 assessment committees

Memberships of Scientific Societies

2021 – Elected Member, *Royal Swedish Academy of Sciences*, Sweden
2007 – *Norwegian Chemical Society,* Norway
2005 – Elected Member, *International Academy of Quantum Molecular Sciences*, international
2005 – Elected Member, *Board World Association of Theoretical and Computational Chemists*
2004 – Elected Member, *Norwegian Academy of Science and Letters*, Norway

Fellowships and Awards

2019 *Nansen Award for Excellence in Science*, Norwegian Academy of Science and Letters
2017 – *Hylleraas Centre of Quantum Molecular Sciences*, director, Centre of Excellence
2017 – 2018 *Centre for Advanced Study*, group leader, Norwegian Academy of Science and Letters
2016 *Ede Kapuy Lecture*, Eötvös University, Budapest, Hungary
2013 *Molecular Physics Festschrift,* Molecular Physics, UK
2011 *ERC Advanced Grant*, EU
2011 *Award for Outstanding Research (Møbius Prize)*, Research Council of Norway
2010 *Research Excellence Award,* ICCMSE, Greece
2007 – 2017 *Centre for Theoretical and Computational Chemistry*, Research Centre of Norway
2007 *Centenary Lectureship and Medal*, Royal Society of Chemistry, UK
2007 *Guldberg–Waage Medal,* Norwegian Chemical Society, Norway
2006 *University of Oslo Research Prize*, University of Oslo
1999 *Charles A. Coulson Lecture*, University of Athens, Georgia, USA
1992 *Golden Spatula*, Chemistry Students' Teaching Award, University of Oslo
1987 – 1989 *Odd Hassel Scholarship*, Research Council of Norway
1985 *Nansen Award for Young Researchers*, Norwegian Academy of Science and Letters

Track Record — Trygve Helgaker

Publications

I have authored or co-authored 356 publications, of which 306 are research articles and 7 are reviews in international journals. These have received more than 26000 citations on Web of Science (24500 excluding self-citations) and 37000 on Google Scholar. My H-index is 76 on Web of Science and 89 on Google Scholar. Four articles have been cited more than 1000 times and 61 articles more than 100 times. In addition, the monograph *Molecular Electronic-Structure Theory* (Helgaker, Jørgensen and Olsen, Wiley, 2000) has been cited more than 3600 times. I have published two translations of Russian fiction to Norwegian. The following are a list of five publications that I consider important (not necessarily most cited), with a short description and the number of citations with/without self-citations.

1. Configuration-interaction energy derivatives in a fully variational formulation,
   T. Helgaker and P. Jørgensen, *Theor. Chim. Acta* **75**, 111–127 (1989)

   In quantum chemistry, most electronic-structure methods beyond Hartree–Fock and Kohn–Sham theory are nonvariationally determined, complicating their mathematical formulation and manipulation. In this and subsequent papers, we showed that such methods benefit from a **Lagrangian reformulation** of the electronic energy, greatly simplifying their mathematical formulation and computation. The Lagrangian technique has become universally adopted for the calculation of time-independent and time-dependent molecular properties. [169/154 citations].

2. Integration of the classical equations of motion on ab initio molecular potential energy surfaces using gradients and Hessians: application to translational energy release upon fragmentation,
   T. Helgaker, E. Uggerud, and H. J. Aa. Jensen, *Chem. Phys. Lett.* **173**, 145–150 (1990)

   This paper presented **on-the-fly ab-initio Born–Oppenheimer molecular dynamics** as an alternative to the Car–Parrinello dynamics, with applications to systems of chemical interest in several follow-up papers. With today's computer power, such studies have now become commonplace. Our implementation was based on a second-order trust-region integration scheme, subsequently implemented in the popular Gaussian code. [230/223 citations].

3. Basis-set convergence of correlated calculations on water,
   T. Helgaker, W. Klopper, H. Koch, and J. Noga, *J. Chem. Phys.* **106**, 9639–9646 (1997)

   The accurate calculation of dynamical electron correlation is a difficult problem, whose solution is needed to reach "chemical accuracy", with errors of about 1 kcal/mol in the calculation reaction energies. Such an accuracy cannot be reached in a brute-force manner, by increasing the basis set used to expand the wave function. In this paper and an equally highly cited follow-up paper, we demonstrated that the correlation energy can be accurately extrapolated from standard calculations, reducing the errors by an order of magnitude at no extra cost. Our **extrapolation method** is still widely used (with more than 100 citations every year), not only for practical calculations but also benchmarking new methods and techniques. [1873/1851 citations]

4. Excitation energies in density functional theory: An evaluation and a diagnostic test,
   M. J. G. Peach, P. Benfield, T. Helgaker, and D. J. Tozer, *J. Chem. Phys.* **128**, 044118 (2008)

   Density-functional theory (DFT) is the workhorse of quantum chemistry, widely used not only for ground-state energies but also for excitation energies. However, the method is not systematically improvable and may fail in manners that are difficult predict. This paper introduces a simple, **inexpensive diagnostic test for the reliability of calculated excitation energies**. The diagnostic is obtained at no cost during the calculation of excitation energies, providing a useful guide to the trustworthiness of the calculated excitation energies. [1061/1057 citations]

5. A paramagnetic bonding mechanism for diatomics in strong magnetic fields,
   K. K. Lange, E. I. Tellgren, M. R. Hoffmann, and T. Helgaker, *Science* **337**, 327–331 (2012)

   In this paper, we discovered a **fundamentally new chemical bonding mechanism**, arising from the interaction of the electrons with an external magnetic field. In a sufficiently strong magnetic field (of the order of 100 kT, as observed on magnetic white dwarfs), these magnetic interactions are sufficiently strong to compete with Coulomb interactions. In particular, covalent bonds are broken by the spin Zeeman interactions but then replaced **paramagnetic bonds** induced by the orbital Zeeman interaction, giving rise to an exotic chemistry not previously suspected or studied. The discovery was made possible by development in our group of a unique quantum-chemistry code for the study of molecules in a magnetic field in a gauge-invariant manner. [85/73 citations].

Major Collaborations

J. Gauss (Mainz) molecular properties, coupled-cluster theory, magnetic fields; *P. Jørgensen* (Aarhus) molecular properties, coupled-cluster theory; *W. Klopper* (Karlsruhe) coupled-cluster theory, high accuracy*; J. Olsen* (Aarhus) molecular properties, coupled-cluster theory; K. Ruud (Tromsø) molecular properties, *A. Savin* (UPMC, Paris) DFT; S. Stopkowicz (Mainz), coupled-cluster theory and strong magnetic fields, *D. Tozer* (Durham) DFT; A. Teale (Nottingham) DFT and strong magnetic fields

Selected invited presentations to peer-reviewed, internationally established conferences:

2019 *Robust optimization of the density in orbital-free DFT*, MQM (Germany)
2018 *Closed-shell molecular paramagnetism*, ICQC (France)
2017 *Quantum chemistry in magnetic fields*, WATOC (Germany)
2016 *CDFT of molecules in weak and strong magnetic fields,* Sanibel (USA) & MQM (Sweden)
2015 *Density-functional theory in magnetic fields*, Pacifichem (USA)
2014 *Exact but differentiable formulation of DFT*, WATOC (Chile) and 248st ACS (USA)
2013 *Molecular magnetism and DFT in magnetic fields*, DFT2013 (UK)
2012 *Chemical bonding in strong magnetic fields*, QSCP (Finland)
2011 *Molecules in strong magnetic fields*, WATOC (Spain) & ISTCP (Japan)
2010 *Ab Initio studies of the adiabatic connection in DFT*, MQM (USA) and EuChemMS (Germany)

I have given 116 oral presentations at conferences and meetings, 25 at workshops, and 73 during visits.

Presentations at international advanced schools:

I have given more than 300 lectures at international advanced schools. Of these, 205 lectures were given at the *Sostrup Summer School of Quantum Chemistry and Molecular Properties*, organized by P. Jørgensen, J. Olsen, and myself biennially 2000–2014. In addition, I have given 65 lectures at the *European School of Quantum Chemistry (ESQC)* biennially 2001–2019 and in 2000.

Major contributions to the early careers of excellent researchers:

I have mentored 19 postdocs (of which 5 now hold permanent faculty positions) and supervised 14 PhD students. Four of my previous group members have won ERC Starting and Consolidation Grants and two have won RCN Young Researcher Talent Grants. I have organized 13 summer schools since 1990 and taught at summer schools every year since 1990. I have written one popular textbook for students (recently reprinted as paperback), with one upcoming book.

Organisation of Scientific Meetings

2020 *Faraday Discussion New Horizons in Density-Functional Theory*, UK, **member**, 190 participants
2019 *Chemistry 2019: On Hassel's Shoulders*, Norway, **member**, 100 participants
2018 *Atoms, Molecules and Materials in Extreme Environments*, Norway, **chair**, 65 participants
2018 *Mathematical Methods in Quantum Chemistry*, Germany, **member**, 45 participants
2018 *Adventures from Num. Quant. Chem. Methods to Biol. Systems*, Norway, **chair**, 70 participants
2017 *50th Anniversary Celebration of IAQMS*, France, **chair**, 60 participants
2016 *Magical Mystery Tour of Electron Correlation*, Norway, **chair**, 70 participants
2015 *Advances in Electronic-Structure Theory*, France, **member**, 104 participants
2015 *Hylleraas Symposium*, Norway, **chair**, 50 participants
2015 *Fundamental Aspects of density-functional theory*, Norway, **chair**, 57 participants
2014 *Promoting Female Excellence in Theor. and Comp. Chem.*, Norway, **member**, 103 participants
2011 *15th European Seminar on Comp. Methods in Quantum Chemistry*, Norway, **chair**, 89 participants
2010 *Quantum Chemistry Beyond the Arctic Circle,* Norway, **member**, 75 participants
2009 *Molecular Properties: Bridging the Gap Between Theory and Appl.*, Norway, **chair**, 94 participants
2007 *A Coastal Voyage of Current Density Functional Theory*, Norway, **member**, 43 participants
2006 *Nanoquant*, Norway, **chair**, 60 participants