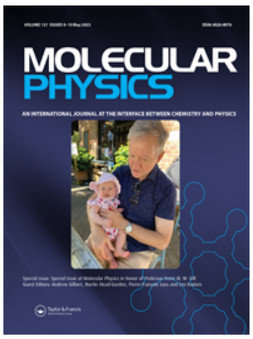

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PETER GILL SPECIAL ISSUE

Introduction to the Peter M. W. Gill special issue

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ABSTRACT
A short scientific biography of Peter M. W. Gill, a prominent theoretical chemist, is reported as the introduction to a collection of manuscripts comprising a Special Issue in his honour.

ARTICLE HISTORY
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KEYWORDS
Quantum chemistry; electronic structure theory; density functional theory

1. Introduction

It is a great pleasure to introduce this collection of invited articles that recognise the scientific accomplishments of our distinguished colleague and friend, Professor Peter Gill, as a slightly late 60th birthday present. We will first summarise a few highlights of Peter's career, in terms of scientific accomplishments, awards and career trajectory, and then add a few personal remarks on our connections to Peter.

2. Research accomplishments to date

Peter Gill is an electronic structure theorist. Electronic structure theory, or quantum chemistry, is the development of methods to approximately solve the time-independent Schrödinger equation. This fundamental equation of quantum mechanics is formally exact but it is unfeasible to exactly solve it for most interesting systems. Therefore, the goal of a electronic structure theorist is to produce useful tools that can be employed to model the structure, relative energies and properties of complex molecules, not just by theorists, but when hardened into practically usable software, by almost any practicing chemist.

Peter Gill's research achievements in quantum chemistry are profoundly significant. Let us begin with a fundamental example. Probably 80% or more of the electronic structure calculations performed today use computer algorithms to evaluate two-electron integrals that Peter has developed – the so-called PRISM approach to matrix element evaluation [1, 2]. Roughly 100,000 chemists, materials scientists, and chemical biologists use these tools every year. The efficient evaluation of molecular integrals has been a reoccurring theme in Peter's research; more recently he developed recurrence relations for three-electron integrals that avoid the resolution of the identity (RI) approximation that is commonly used [3]. Only 5 years ago he produced a brilliant new algorithm for the evaluation of matrix elements involving effective core potentials [4] which is fully analytic, in contrast to the semi-numerical methods that are standard today, with associated limitations in precision and efficiency. Thus Peter is a world leader in the methods that lie literally at the core of computational chemistry software.

There are numerous other critical advances in quantum chemistry that Peter has pioneered. First, as a postdoc in the 1990's, Peter led the introduction of systematic, well-defined density functional theory (DFT) procedures into chemistry, together with his postdoctoral advisor, John Pople [5–10]. Nowadays, DFT methods are the most widely used electronic structure methods in chemistry, as well as allied fields. Within density functional theory, Peter solved the problem of the uniform electron gas subject to a range-separated Coulomb potential (i.e. where it is split into a smooth term that is long-range, and a short-range term with a cusp in the zero-distance limit) [11]. Use of range-separation has subsequently become profoundly important in DFT (most of today's best hybrid density functionals use range-separation) [12], and Peter's research helped make this paradigm shift possible. More recently, Peter has explored the development of exact solutions to the Schrödinger equation for different types of finite uniform electron gases that are confined to rings ('ringium'), spheres ('spherium') or

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glomes ('glomium'). This beautiful sequence of papers [13–15], produced in close collaboration with Pierre-François Loos (co-editor), can be enjoyed entirely at an intellectual level, but also provides potential inspiration for future density functionals by providing alternative reference solutions for which a uniform electron gas of a different type is exact [16–18].

Peter Gill is widely recognised for the development of other important algorithms in quantum chemistry, that have enormous practical significance. Peter developed early linear scaling methods [19–21] (including with Martin Head-Gordon [22] (co-editor)) that assemble the DFT effective Hamiltonian to permit us to perform calculations on large molecules with no loss of accuracy. These algorithms have also made their way into multiple quantum chemistry codes. Another example is the development of the Maximum Overlap Method (MOM) [23–26] together with Andrew Gilbert (co-editor). The MOM facilitates the convergence of self-consistent-field methods (SCF) to higher-energy solutions of the Hartree-Fock or Kohn-Sham equations, thus allowing ground-state algorithms to be applied to excited states. This work has important implications for efficiently evaluating low-lying excited states of large molecules, as well as exotic states, such as core-excitations relevant to NEXAFS and XAS spectroscopy.

In addition to these high-impact successes, Peter has also produced beautiful and exciting advances on very difficult, fundamental problems in quantum chemistry that are not yet as well-recognised. This includes work on so-called intracules [27–41], on new resolutions of the Coulomb operator [42–48], on novel ways to compute the second-order Møller-Plesset energy [49, 50], and discovering the chemistry of one-dimensional systems [51–54]. The scope of his publications demonstrates Peter is not just a chemist, but also a mathematician *par excellence*! [55–57].

3. Career and recognition

A New Zealander by birth, Peter Gill obtained B.Sc. and M.Sc. degrees from the University of Auckland in 1983 and 1984. After crossing the Tasman, Peter obtained his Ph. D. from the Australian National University in 1988, working with Prof. Leo Radom (co-editor). His Ph. D. delved into hemi-bonding as well as convergence of perturbation theory. Between 1988 and 1993, Peter performed postdoctoral research with 1998 Nobel Laureate Sir John Pople, at Carnegie-Mellon University in Pittsburgh, USA, which launched his interests in two-electron integral evaluation and density functional theory. Here Peter met Martin Head-Gordon, then a student with Pople, for the first time upon his arrival at Pittsburgh airport where he correctly deduced that he must be the person holding the $\hat{H}\Psi = E\Psi$ sign.

Peter's independent career commenced in 1993 when he accepted a lectureship at Massey University (New Zealand), followed by a lectureship at the University of Cambridge in 1996. Only 3 years later, Peter became the inaugural chair of theoretical chemistry at the University of Nottingham, where he stayed for 5 years before accepting a professorship at the Australian National University. Most recently, Peter moved again in 2019 to his current position, the Schofield Chair in Theoretical Chemistry at the University of Sydney.

In software development, Peter's postdoctoral research was crucial to the introduction of DFT into the widely used Gaussian programs. At the end of 1992, Peter co-founded the Q-Chem software package to which he and his group have made many important contributions. Indeed, for over 20 years, between 1998 and 2020, Peter was the President of Q-Chem Inc. The stories of its scientific development are contained in a series of major reviews [58–63]. Less easy to learn about is the fact that Peter is a first-rate leader, one who is able to build consensus, and also take the lead directly when necessary.

Peter has performed significant service to scientific associations and has been elected to several scientific societies and academies of special relevance to theoretical chemistry. Peter was elected as a Fellow of the Royal Australian Chemical Institute (2009), the vice-president of the International Society of Theoretical Chemical Physics (ISTCP) (2009), a fellow of the Australian Academy of Science (2014), a member of the International Academy of Quantum Molecular Science (IAQMS) (2015), the president of the World Association of Theoretical and Computational Chemists (WATOC) (2017) and the vice-president of the Asia-Pacific Association of Theoretical and Computational Chemists (APATCC) (2019).

Peter's scientific accomplishments have also been recognised with a range of relevant awards, commencing with the Dirac Medal of WATOC (1999); the Pople Medal of APATCC (2005); the Schrödinger Medal of WATOC (2011); the Fukui Medal of APATCC (2013); the Biennial Medal of the Association of Molecular Modellers of Australasia (2014); and the David Craig Medal of the Australian Academy of Science (2019).

4. Concluding thoughts

Peter's published works are testament to his scientific prowess, but those of us who had opportunities to interact with him personally can also testify to his many positive traits that make him not just a scientist, but a great one.

Peter has an ability to clearly communicate ideas which is exemplary, and makes his presentations

favourites among students at lectures, and fellow scientists at conferences. When speaking he is cognisant of his audience and endeavours to convey his message with a clarity and simplicity that would make William of Ockham proud.

Peter has a meticulous attention to detail, an attribute that can be initially frustrating for an eager student, but ultimately instils a discipline in both thought and writing. One of us recalls a discussion about whether a 10^{-50} E_h violation of the variational theorem was indicative of a bug in the code. It was.

Peter is creative and not afraid to think outside the box when it comes to developing new approaches in quantum chemistry. This is evidenced by his work on intracules, one-dimensional systems, finite uniform electron gasses and even proposing a new unobserved observable [64]. It is scientists with a vision like his that will allow our subject to take the next giant leap forward.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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