Perdew Festschrift editorial

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This special issue of the Journal of Chemical Physics is dedicated to the work and life of John P Perdew. A short bio is available within the issue[1]. Here, we briefly summarize key publications in density functional theory by Perdew and his collaborators, followed by a structured guide to the papers contributed to the special issue.

The first part of this editorial focuses on the work of John Perdew himself, with a special emphasis on some of his more important papers. That work fits into two categories. In the first category, there are the approximations he has developed, often with several co-authors. These approximations are so heavily used that Perdew is likely the most cited physicist of all time. The second category focuses on his more foundational and conceptual works. These derive many properties of the exact functional, and influence how we think about it. They have had enormous influence in the entire community of DFT developers, whether in chemistry or physics or elsewhere.

I. DENSITY FUNCTIONAL THEORY AND JOHN PERDEW

Density functional theory (DFT) is an enormous success story. In particular, Kohn-Sham density functional theoryi (KS-DFT)[2,3] is the world's most popular electronic structure method. From about 1965 to 1990, it was the standard tool for solid-state electronic structure calculations. About 1990, better approximations made it usefully accurate in chemistry, leading to a revolution in quantum chemistry, and finally the Nobel prize in chemistry to Walter Kohn and John Pople in 1998.

John Perdew is the physicist who has done more than any other to develop both the theory and approximations used in DFT calculations. Because of this, Perdew is (very likely) the most cited physicist of all time. Fig 1 shows citations to his papers over time, as computed by web of knowledge. The scale is in thousands of citations per year. The enormous numbers largely reflect the many approximations which he developed that are in common use today. In particular, almost all materials calculations using DFT (which is almost all of them) use an approximation bearing his name (or, at least, initial). NERSC estimates that about 30% of DOE's entire supercomputer is devoted to DFT calculations and almost all use one or another of Perdew's formulas.

Fig 2 also shows how remarkably productive Perdew has been, as it shows the number of papers each year, since 1976, i.e., during almost half a century. Even today, at age 80, he remains remarkably productive and active. The dip for 2023 likely reflects his moving to a new faculty position at Tulane, which is also a return home[1]. We are confident his pace will pick back up in future years.

Perdew is most well-known to the world for the number and impact of his approximations (often in collaboration) for the XC energy. The *Self-interaction correction to density-functional approximations for many-electron systems*, with Alex Zunger in 1981[4] combined deep insights with a very practical approximation, the self-interaction correction (SIC). An entire subfield of DFT has evolved in 40 years and uses SIC for some of the most difficult materials problems[5].

A key input to the local density approximation (LDA) is the XC energy per particle of the uniform electron gas[3]. The paper above contains an early version (PZ81) of this XC energy that is used in many LDA calculations. A later update was *Accurate and simple analytic representation of the electron-gas correlation energy*, with Yue Wang in 1992[6] (PW92).This yeoman's work provided the most careful and accurate formula for the uniform electron gas energy, a vital input into almost all DFT approximations used in materials science.

Perdew's most heavily cited work is for the development of generalized gradient approximations (GGAs). This work spanned about 20 years, starting in 1977 with the formal work with David Langreth[7]. With many papers along the way, this led to *Generalized gradient approximation made simple*, with Ernzerhof and Burke in 1996 (PBE).[8] This is the most cited Physical Review Letter ever. It was based on general principles of quantum mechanics, and used no empirical input. The paper showed that seven simple exact constraints yield the same approximation as a fully numerical construction from many-body heory[9]. This approximation is the most commonly used for materials calculations and is the driver behind the materials genome project and about 30% of all DOE supercomputer use.

Other variations (some earlier, some later) also exist, including the *Density-functional approximation for the correlation energy of the inhomogeneous electron gas* in 1986 (P86).[10]. This early generalized gradient approximation is

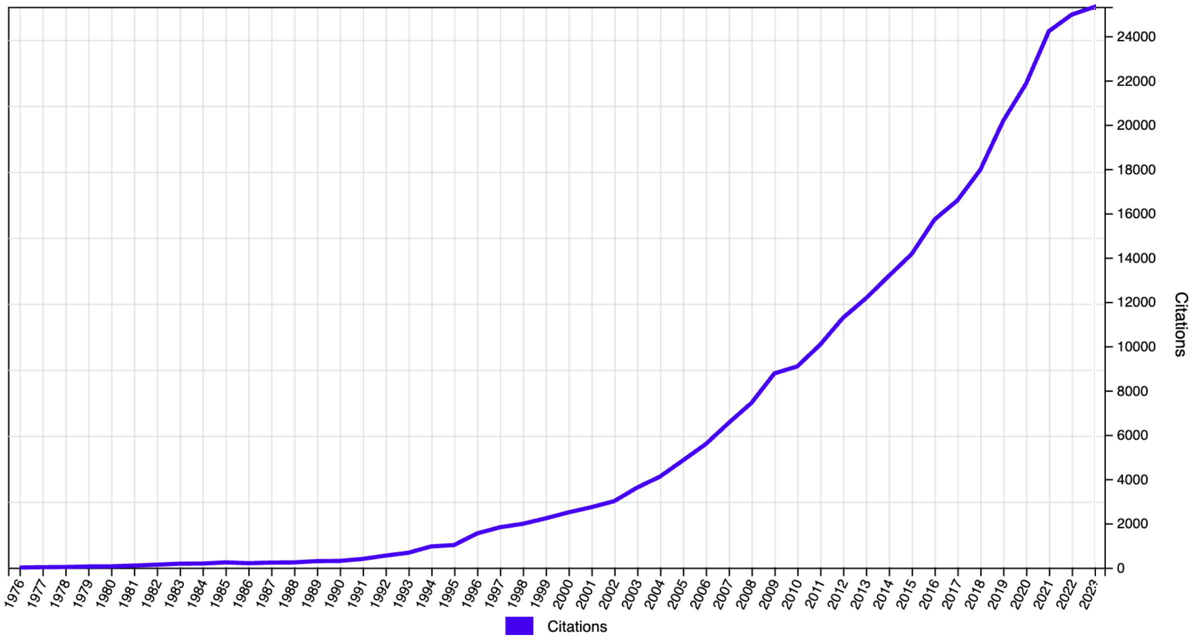

FIG. 1. Number of papers citing Perdew's work each year from 1976 to 2023

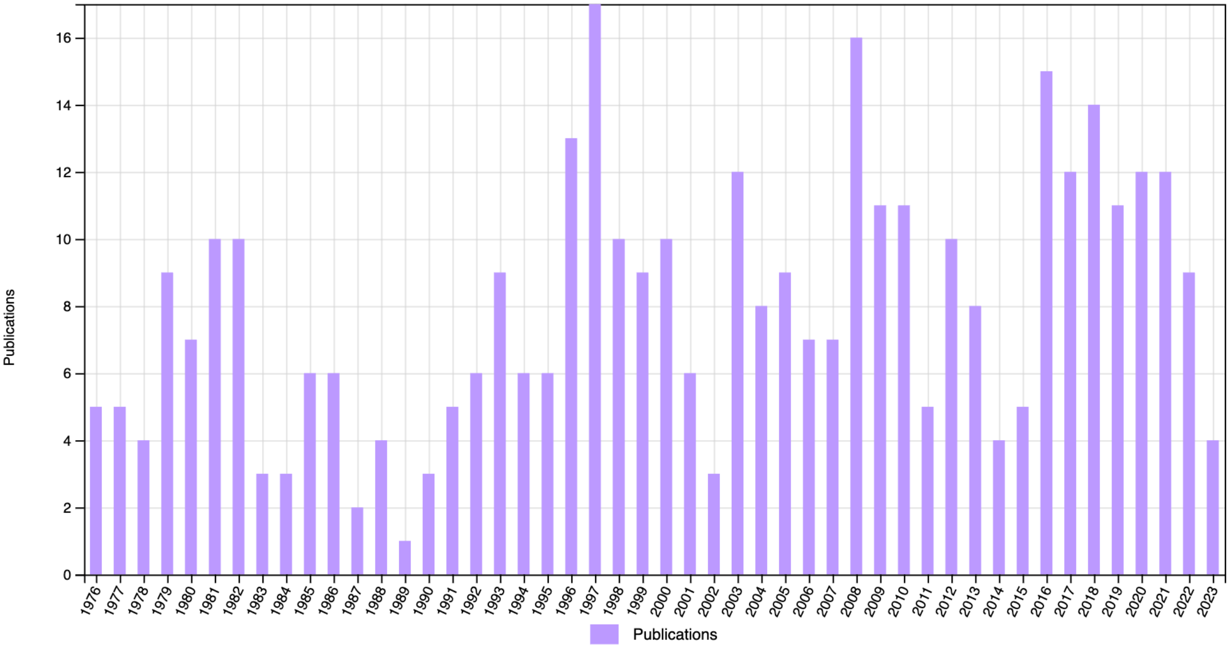

FIG. 2. Number of papers published by Perdew each year from 1976 to 2023

still in considerable use today, especially when weak non-covalent bonds are important. A later variant was tested in *Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation*, with many co-authors (1992)[11]. This is the famous PW91 approximation[12], the precursor to the ubiquitous PBE, and still in common use today. On the other hand, one could later see the limitations of the PBE functional for lattice parameters and phonons, leading to *Restoring the density-gradient expansion for exchange in solids and surfaces* with many co-authors in 2008 (PBEsol)[13]. This modification of the PBE generalized gradient approximation was designed to improve properties for solids, while lessening accuracy for energy differences. It has become a standard alternative to PBE for solid calculations of lattice constants and phonon spectra.

The meta-GGA is the next logical step after GGA's in improving semilocal functionals. The *Strongly constrained and appropriately normed semilocal density functional* with Sun and Ruzsinszky in 2015 (SCAN)[14] meta-GGA is the latest version from Perdew and co-authors, and does almost everything better than PBE. It is being widely adopted by the materials community. Finally, we mention global hybrids, functionals that mix in a fixed fraction of exact exchange. *Rationale for mixing exact exchange with density functional approximations* with Ernzerhof and Burke in 1996[15] shows how mixing 1/4 of exact exchange could be theoretically justified, and led directly to the creation of PBE0.

However, perhaps somewhat less well known to the community of DFT users, but equally important, are his contributions to the fundamental theory behind DFT. Many of these prove exact conditions that the exact functional must satisfy. These then form crucial building blocks for the design of his most successful approximations.

Despite its odd name, *The exchange-correlation energy of a metallic surface*, with David Langreth in 1975[16] was the first to correctly identify the adiabatic connection - fluctuation dissipation formula in KS-DFT. This method for analyzing exact and approximate functionals is now part of all textbooks on the subject. Some of our most important insights into global hybrid approximations are due to this result[17].

Another key paper involves deriving exact conditions. *Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms*, with Mel Levy in 1985[18] was the first precise use of coordinate scaling to derive many of the exact conditions that guide non-empirical functional construction today. In particular, almost all new approximations for exchange satisfy their simple relation.

Perhaps the most celebrated (and subtle) paper concerns variations with particle number. *Density-functional theory for fractional particle number: Derivative discontinuities of the energy*, with Levy, Parr, and Balduz in 1982[19] extended the domain of DFT to fractional electron numbers based on the grand canonical ensemble, and developed the exact conditions for fractional electron numbers. It clearly identified the infamous derivative discontinuity of the exact energy functional for the first time, and showed how the Kohn-Sham band gap of a periodic solid is an underestimate of the fundamental gap, even with the exact XC functional.

The rest of this editorial is a discussion of the many various papers in the rest of this issue. Almost every DFT paper published today contains some nugget of Perdew's work, and about half of them cite him.

II. GUIDE TO PAPERS IN THIS SPECIAL ISSUE

As you will see in the contents of this special issue, KS-DFT is applied to a dazzling array of diverse problems, and folks are working in many different directions to improve it. We have done our best to provide a structured guide to the contents.

A. Exact Conditions, limits, bounds, and prototypical systems

Several of the papers focus on the development or understanding of conditions satisfied by the exact functional. Laestadius et al[20] revisit the exchange-only virial relation[18] from the adiabatic connection. Pederson and Burke[21] consider if local conditions have been overenforced in guiding density functional approximation, and if that might explain the quite strong difference between approximations used in materials and those used in chemistry. On the other hand, Burgess et al[22] consider the convexity condition, i.e., that the total energy as a function of particle number is a convex function[19], and give an extremely general proof. Ayers[23] shows by explicit construction that the energy is not a convex function of the number of particles for the Coulomb-like r^{-k} repulsion with $k > log_3 4$. In a completely different vein, Sobrino et al[24] look at a very simple lattice Hamiltonian, and show how it is related to DFT in real space, especially at finite temperatures[25]. Savin and Karwowski[26] revisit the adiabatic connection formula[16], generalizing it beyond first order perturbation theory. Redd et al[27] investigate the exchange energy of neutral atoms in the large-Z limit while Daas et al[28] investigate the large-Z limit of neutral atoms for both exchange and infinite-coupling strength interaction. Lin et al[29] calculate the coupling-constant averaged exchange correlation hole of the 2-electron Hooke's atoms and study the effect of electron-electron cusp condition.

B. Tools

John Perdew has always been an important developer of tools for understanding DFT. Gould[30] has taken basic concepts from density-corrected DFT[31] and applied them to the Hartree case, i.e., where the XC energy is set to zero, to measure differences between densities. On the other hand, Lutz et al[32] have applied tools from conceptual DFT (as championed by Bob Parr[33]) to study hydrolysis reactions of various metal hexafluorides, while Titeca et al[34] extend the charge stabilization method from conceptual DFT to include the Fukui function and electron localization function in combination of Berlin's binding function for studying the dissociative electron attachment (DEA) mechanism in ethene and its chlorinated derivatives. Roy et al[35] develop an electron-centric approach to calculating the XC energy directly, without needing an explicit density functional. Tozer[36] revisits some old ideas of Ghosh and Parr concerning the scaling of the functional under density scaling[18]. Finally, Zhang et al[37] use the Pauli energy to characterize if bonds are weak or strong.

C. Beyond ground-state KS-DFT

Most (but not all) of Perdew's work has focused on developing ground-state Kohn-Sham DFT, where indeed most of the applications of DFT occur. But ground-state DFT directly yields only ground-state quantities, so excitations and other properties require extensions, such as time-dependent DFT[38]. Another kind of extension is to use other techniques from more traditional many-body approaches, which typically yield both ground-state energies and other useful properties, such as the spectral function[39].

Sigurdson et al[40] study Rydberg states of molecules, but include the self-interaction[4] correction to improve KS potentials. Darwood and Maitra[41] show how to find an improved description of double excitations within TDDFT, while Kaplan and Ruzsinszky[42] study the other extreme of low-energy excitations in a uniform gas. Tang et al[43] use many-body theory to study K-edge spectroscopy in salt solutions. Fang et al[44] use TDDFT to study both excitations and ultrafast dynamics in porphyrins.

On the other hand, Wei et al[45] show how to calculate dissociation of H_2 on a copper surface via an embedding technique using the random phase approximation (RPA). Graf and Thom[46] claim that RPA energies can be improved by using HF densities using DC-DFT.

Simplified Hamiltonians are the mainstay of condensed matter physics. Dutta et al[47] develop an efficient algorithm to implement the recently introduced binary tree state (BTS) ansatz on a classical computer, which shows great promise in benchmark applications to the reduced Bardeen-Cooper-Schrieffer Hamiltonian and the one-dimensional XXZ Heisenberg Hamiltonian. Adhikari and Baer[48] develop first and second-order solvers for the Itô-Schrödinger equation using the Itô-Taylor expansion with exact derivatives in the interaction picture, which proved efficient on thermal-coupled Morse oscillators, yielding practical estimates within tens of iterations.

Returning to DFT, Yu et al[49] show that the underdetermination problem to define a ground-state energy functional of the natural determinant reference (NDR) are overcome in a grand-canonical ensemble framework at the zero-temperature limit, while Harding et al[50] propose a generalized thermal adiabatic connection (GTAC) formula that uses a fictitious temperature parameter to improve simulations of warm dense matter.

D. Approximations

A large number of our papers are devoted to the development of new DFT approximations and their testing. We classify these based on the level of approximation that's being tested, trying to follow Jacob's ladder[51].

Going all the way back to the HK theorem, in orbital-free DFT, Horowitz et al[52] study orbital-free DFT for metal slabs. At the level of pure exchange, Bosko and Satroverov[53] revisit the Fermi-Amaldi approximation for exchange, the original inspiration for the SIC correction, while Trushin and Görling[54] discuss how to do exact exchange calculations for open shell systems. Then Aschebrock et al[55] show that the ultra-nonlocal density response of exact exchange can be accurately captured by a metaGGA.

In terms of global hybrids, the work of Hostas et al[56] discusses how the fraction of exact exchange greatly affects ordering of spin states in a transition metal cluster, as do Manukovsky et al[57].

Much work is now focussed on meta-GGAs. Francisco, Cancio, and Trickey[58,59] have contributed two papers on the Tao-Mo meta-GGA functional (not a Perdew approximation): The first simplifies it, while the second removes its explicit orbital-dependence, a vital step if it is to be used in an orbital-free code. Kovacs et al[60] discuss in general how metaGGA's affect band gaps in solids. Meanwhile Palos et al[61] use density corrected DFT to study ion hydration in water using SCAN. Wittmann[62] use the SCAN variant, r^2SCAN, to construct several global double hybrid approximations.

There is also much interest in treating strongly correlated systems, and using more non-local ingredients. Constantin et al[63] revive the interaction strength interpolation (ISI) of Perdew and co-workers[64], generalizing old forms to better fit the adiabatic connection of the uniform gas. Meanwhile, Shi et al[65] use partition DFT to introduce approximations that capture effects in strongly correlated systems, while Ponra et al[66] look at difficult multireference cases and how the muliplet-sum-method treats them. Chen and Yang[67] develop a machine-learning finite-range nonlocal density functional. In a totally new vein, Tancogne-Dejean et al[68] propose to replace the energy functionals in ground-state DFT with exact, physically equivalent force formulations. Zhang et al show that commonly used density functionals struggle to accurately simulate the structural, electric, and magnetic transitions of VO_2 from insulating to metallic phases.

An important class of functionals for molecular calculations is the double hybrid. Becke[69] presents some slight but crucial revisions to the DH23 hole-based functional, slightly reducing its error, but also showing better generalization, managing a record-breaking 1.76 kcal/mol error for the (weighted) mean absolute deviation on the GMTNK55 database. Meanwhile, Bi et al[70] explore the effect of the choice of density in XYG3-type double hybrids, and Bremond et al[71] introduce a new flavor of range-separated double hybrid and test its properties for both ground states and excitations.

In terms of self-interaction corrected functionals, Bi et al[72] introduce a novel constraint that facilitates self-consistent localization of the self-interaction-correction orbitals to solve its well-known numerical instability. Tancogne-Dejean et al[73] extend some of the well-established self-interaction correction (SIC) schemes of density-functional theory — the Perdew-Zunger SIC and the average-density SIC — to the case of systems with noncollinear magnetism. Hooshmand et al[74] explore the reasons why standard functionals fail for diradical systems, and the improvements that can be found with self-interaction corrections. Singh et al[75] investigate the reasons behind the improvement in chemical reaction barrier height predictions by the Fermi–Löwdin orbital self-interaction correction (FLOSIC)[76]. Manier et al[77] show that while LSDA and PBE effectively describe the strongly correlated chromium dimer by breaking spin-symmetry , a full Perdew–Zunger SIC creates an unphysical symmetry-broken state.

For weakly bonded systems, Ning et al[78] show the importance of van der Waals (vdW) and self-interaction corrections for accurate first-principles cuprate lattice dynamics.

Lastly, the work of Lehtola and Marques[79] is about *all* modern XC approximations. They curate the libXC library of approximate functionals, and their paper is a plea to those suggesting new approximations, and how to avoid ambiguities when reporting them.

E. Calculations

Although you could never tell from this special issue, at least 90% of all papers using DFT simply report the results of KS-DFT calculations in order to compare with experiment and do some science. In this section, we discuss the papers that are primarily focussed on that. It gives a nice sense of the breadth of modern DFT applications.

For materials science, Rumson and Johnson[80] study the thermal expansion of layered electrides and the importance of the approximation used. Ramakrishnan and Jain[80] attempt to estimate band gaps of various semiconductors using reference calculations with the HSE06 functional[81]. Yang et al[82] study irradiation effects in silicon transistors using TDDFT calculations to find excitations. Machrodt et al[83] calculate the energies and charge and spin distributions of the low-lying excited states in singlet and triplet N_2V defects in diamond from direct Δ-SCF calculations with various density functionals. Remsing and Thakur[84] study the Nuclear quantum effects in the acetylene: ammonia plastic co-crystal. Liu et al[85] assess the r2SCAN meta-GGA for structural parameters, cohesive energy, mechanical modulus, and thermophysical properties of 3d, 4d, and 5d transition metals. Friedrich and Curtarolo[86] provides the AFLOW with the coordination corrected enthalpies (CCE) method for the thermodynamics of ionic materials.

In terms of chemistry, Petersen and Solling[87] report how small halocarbons dissociate, a crucial question in destruction (or recovery) of the ozone hole in the upper atmosphere. Pederson et al[88] use Fermi-Löwdin orbitals (FLO) for self-interaction corrections (SIC) in DFT calculations of anion-solvent interactions. Nguyen et al[89] show that the FLO self-interaction correction can reproduce the bond-length alternation in π-conjugated polymers. Chen et al[90] use the XYG3 approximation to create a global potential energy surface for Al and O_2.

Finally, several papers focus on the importance of basis sets in all these calculations. Determan and Wilson[91] design correlation consistent basis sets for density funcitonal calculations, focusing on the third-row atoms (Ga-Br). Yang et al[92] develop correlation-consistent numeric atom-centered orbital basis sets for Krypton with applications in RPA-based correlated calculations.

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We end by thanking John Perdew for his endless source of ideas, his endless inspiration and perspiration in pursuing them, and his general all-round good humour that permeates this field and community. We hope that readers will find this Festschrift special issue useful and we look forward to celebrating his 100th birthday. We also point out, for the sake of Perdew's many collaborators over the years (including the three of us), that the middle initial P could stand for pesky, persnickety, or pnitpicky. Take your pick.

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