Louisiana EPSCoR

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Tulane physicist receives top honors for theories on "nature's glue"

Tulane University physics Professor John P. Perdew was elected to the National Academy of Sciences (NAS) in May 2011 for his key role in the development of density functional theory (DFT). Dr. Perdew joins the NAS ranks with LSU physicist Dr. Ward Plummer, who was elected in 2006, and 2,100 other distinguished scientists, many of which are Nobel Prize winners. Drs. Perdew and Plummer are members of the Louisiana Alliance for Simulation-Guided Materials Applications (LA-SiGMA), funded by NSF EPSCoR.

The NAS was established by President Abraham Lincoln to recognize leading scientists in all fields and to provide science advice through reports to the Federal government. New members are chosen by member vote and being elected to the NAS is one of the highest honors for a scientist or engineer.

The NAS election citation says, "Perdew has led the effort to put a sound mathematical and physical foundation under the conceptual ideas of Density Functional Theory. Perdew derived exact properties of the exchange-correlation energy, using exact constraints to construct the approximations widely used for applications across condensed matter physics, chemistry, and materials science."

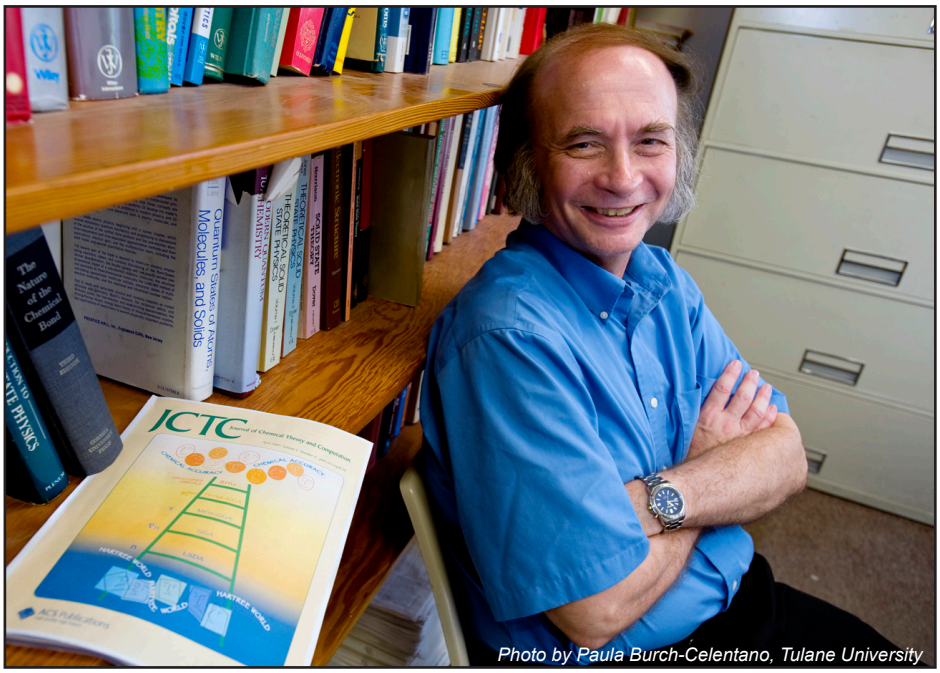

Photo by Paula Burch-Celentano, Tulane University

The April 2009 issue of the American Chemical Society's Journal of Chemical Theory and Computation (JCTC) was dedicated to Dr. John Perdew to honor his career and contributions toward the development of density functional theory. Dr. Perdew is one of LA EPSCoR's lead investigators in the NSF-funded materials science research alliance, LA-SiGMA.

So, what is DFT?

The material world is made up of atoms, molecules and solids, which in turn are made of electrons and nuclei. The nuclei provide the forces that hold the electrons together, but the electrons are quantum mechanical particles that repel one another. With these fundamental interactions, scientists have long wondered what atoms, molecules, and solids can exist, and with what shapes and properties? Before 1965, these questions could only be roughly answered.

Dr. Perdew further explains: "DFT provided a way to get accurate answers more efficiently by solving one-electron wave equations with selfconsistent effective potentials. The theory was exact in principle for the state of lowest energy, and approximate but improvable in practice. The improvements, to which I and others contributed, as well as advances in computer hardware and software, led to the adoption of this theory in chemistry and to the 1998 Nobel Prize in Chemistry, shared by physicist Walter Kohn (for DFT) and chemist John Pople (for sophisticated computer codes). Nowadays, DFT is applied largely through powerful standardized computer codes.

The way to make DFT more accurate was to improve its approximation for the electron-density-dependence of its exchange-correlation energy, which is responsible for most of the binding of one atom to another. So I and others have been guessing the rule for "nature's glue", guided by the exact conditions that we and others had derived. I was lucky to find at Tulane a brilliant long-term collaborator in Dr. Mel Levy (Chemistry). And I have had many other outstanding junior and senior collaborators, here and elsewhere."

> "Neither my postdoctoral supervisors who introduced me to DFT nor I could have anticipated that this theory would become the most widely-used and widely-cited theory of the past thirty years, playing a key role first in condensed matter physics, then also in chemistry, and now also in geosciences and engineering."
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> *- Dr. John P. Perdew, Tulane University*

A World Leader in Citations

Journal citations are a key indicator of the impact of a scientist's work. Last year, Tulane University physics and math student Alan Liu ran reports on the most-cited researchers listed by information company Thomson Reuters. Liu discovered that nearly 70,000 citations refer to Dr. Perdew's work on DFT, ranking him as the world's most cited physicist from 1981-2010.

In response to the report, Dr. Perdew humbly replied, "My co-authored papers that appear on this list do so because they provide widely used approximate functionals for electronic structure calculations. An article's potential for citedness depends strongly on the population of researchers in its field and sub-field. Even within a sub-field, the most cited papers are not always the best ones."

Luck Has Played a Role

According to Dr. Perdew, he attributes "luck or unseen help" as a major factor in the launching of his career success, as it had a bit of a rocky start.

When Dr. Perdew completed his Ph.D. from Cornell University in 1971, the job market for academic physicists was at an all-time low. He spent six years working in temporary post doctoral research positions. This felt like the worst luck, however, he now realizes that it was good luck in disguise.

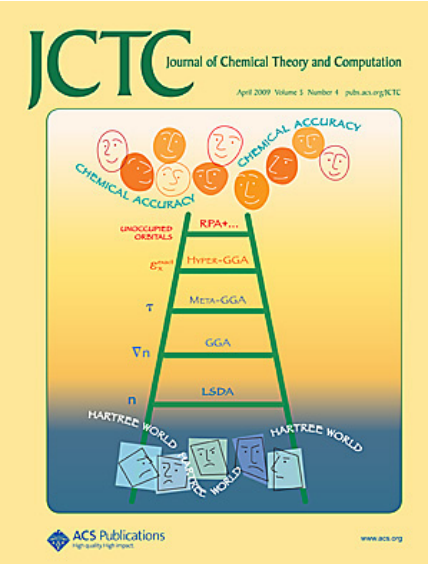
By the time he was hired as an assistant professor at Tulane University, he had worked with Dr. Sy Vosko at Toronto and Dr. David Langreth at Rutgers, both of whom were fundamentally interested in the DFT of electronic structure that had been proposed in 1964 by Hohenberg, Kohn, and Sham.

"This theory was showing a few early successes in solid state physics at the time my postdoctoral supervisors introduced me to it. Neither my postdoctoral supervisors who introduced me to DFT nor I could have anticipated that this theory would become the most widely-used and widely-cited theory of the past thirty years, playing a key role first in condensed matter physics, then also in chemistry, and now also in geosciences and engineering," said Perdew.

"So the bad luck of not finding a permanent job for six years was also the good luck of getting in on the ground floor of a powerful new theory. And when the Tulane Physics Department hired me, they gave me the freedom and security to develop this theory further over many years," added Perdew.

Research Refinements

Dr. Perdew's research has been supported steadily by the NSF since 1978, and more recently also by LA-SiGMA. The LA-SiGMA alliance, which includes prominent researchers from seven Louisiana universities, LA EPSCoR, and the LA Board of Regents, is leveraging a 5-year NSF grant to transform research and education in computational materials science in Louisiana.



The cover of the JCTC journal honoring the career of Dr. Perdew depicts the "density functional theorist's dream and expectation of building more accurate exchange-correlation density functionals based on careful consideration of physical principles and exact constraint imposition."

Perdew's LA-SiGMA research team will continue to develop more accurate functionals that will be turned into high-performance computational codes by the LA-SiGMA Cybertools and Cyberinfrastructure (CTCI) team. The resulting codes will be used to advance the research of all of the LA-SiGMA science drivers, which include multiscale methods for strongly correlated materials, materials for energy storage and generation, and biomolecular materials.

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