# Rensselaer

The Department of Physics, Applied Physics and Astronomy

*Gail and Jeffrey L. Kodosky '70*
*Distinguished Lecture Series in Physics*

Presents:

Dr. John P. Perdew
Departments of Physics and Chemistry
Temple University

Wednesday, March 1, 2017
4:00 pm – DCC 324
(Refreshments at 3:30 pm)

## "Density Functional Theory for Materials Discovery: Systematic Approximation and the SCAN Functional"

Discovery of useful or interesting new materials and molecules by computation requires an efficient, accurate, and reliable theoretical method, and the preferred method is still Kohn-Sham density functional theory[1]. In this theory, the exact ground-state energy and electron density (and thus the nuclear positions) can be found by solving self-consistent one-electron equations. The exchange-correlation energy as a functional of the electron density must in practice be approximated. I will discuss a systematic and proven way to improve the approximations, making them more accurate and reliable at a modest increase of computational cost. Then I will show how this approach has led to SCAN [2], a strongly-constrained and appropriately normed functional that, without being fitted to any bonded system, makes accurate predictions for diversely-bonded materials and molecules [3].

[1] W. Kohn and L.J. Sham, Self-Consistent Equations Including Exchange and Correlation Effects, Phys. Rev. **140**, A1133 (1965).
[2] J. Sun, A. Ruzsinszky, and J.P. Perdew, Strongly Constrained and Appropriately Normed Semi-local Density Functional, Phys. Rev. Lett. **115**, 036402 (2015).
[3] J. Sun, et al., Accurate First-Principles Structures and Energies of Diversely-Bonded Systems from an Efficient Density Functional, Nat. Chem. **8**, 831 (2016).



John P. Perdew is the Laura H. Carnell Professor of Physics and Chemistry at Temple University. His research in the density-functional theory of electronic structure has helped to establish this theory as the most widely-used method to predict the properties of atoms, molecules, and solids from the principles of quantum mechanics. According to *Nature (2014)*, he co-authored two of the 100 most-cited scholarly articles of all time in all fields. He was elected to the National Academy of Sciences in 2011, and received the Materials Theory Award of the Materials Research Society in 2012, a Humboldt Research Award in 2014, and the John Scott Medal in 2015. Perdew directs the Energy Frontier Research Center at Temple.

## Gail and Jeffrey L. Kodosky '70

Jeff Kodosky received a BS degree in Physics from Rensselaer in 1970. He is Co-founder, Director, and Fellow at National Instruments, a leading developer and manufacturer of integrated software and hardware for engineers and scientists. LabVIEW, co-created by Kodosky, is the industry-standard graphical programming environment for measurement and automation. Jeff is a Trustee of Rensselaer since 2002. Gail is a native of Troy, NY and is a retired administrative assistant. Gail and Jeff live in Austin, TX and have two daughters and four grandchildren.