DREXEL UNIVERSITY
Materials Science and Engineering
College of Engineering

Department of Materials Science and Engineering
Winter Seminar Series

3:00 PM, Wednesday, March 8
PISB 104

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

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Abstract: 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).

Bio: John Perdew received his Ph.D in physics from Cornell University in 1971. He was a postdoc at the University of Toronto and at Rutgers University. In 1979 he joined the faculty at Tulane University as Assistant Professor of Physics. He became Full Professor in 1982. In 2013 he moved to the College of Science and Technology at Temple University as the Laura H. Carnell Professor of Physics and Chemistry. He is the founding director of the Center for Materials Theory at Temple.

The National Academy of Science 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 material science". His work on density functional theory has made him one of the world's most cited phycisists. Professor Perdew has five co-authored works among the 11 most-cited physics papers published 1981-2010, and two among the 100 most-cited scholarly articles of all time (Nature **514**, 550 [2014]).

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