Temple University Mathematics Colloquium

John Perdew

Temple University, Department of Physics

will speak on

Climbing the Ladder of Density Functional Approximations

ABSTRACT: Kohn-Sham density functional theory is the most widely-used method of electronic-structure calculation in materials physics and chemistry, because it reduces the many-electron ground-state problem to a computationally tractable self-consistent one-electron problem. Exact in principle, it requires in practice an approximation to the density functional for the exchange-correlation energy. Common approximations fall on one of the five rungs of a ladder, with higher rungs being more complicated to construct but potentially more accurate. The first three or semi-local rungs are important, because (a) they are computationally efficient, (b) they can be constructed non-empirically, and (c) they can serve as input to fourth-rung hybrid functionals. The third-rung meta-generalized gradient approximation can recognize and describe covalent, metallic, and weak bonds, providing a good description of the equilibrium properties of many molecules and solids.

Typically, the non-empirical construction of a density functional approximation proceeds by satisfying exact constraints on the density functional for the exchange-correlation energy, some of which have been derived by mathematicians. Further constraints, including a tighter lower bound on the exchange energy, could be helpful.

Monday, September 16, 2013
Lecture at 4:00 pm
Coffee, tea, and refreshments from 3:40 pm
Room 617, Wachman Hall
Department of Mathematics