

COLLOQUIUM

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Walter Kohn and the Creation of Density Functional Theory

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Abstract:

The theoretical physicist Walter Kohn was awarded one-half the 1998 Nobel Prize for Chemistry for his mid-1960's creation of an approach to the many-electron problem in quantum mechanics called density functional theory (DFT). DFT establishes that the ground state charge density provides a complete description of ALL the properties of any atom, molecule, or solid. This was a breakthrough (both conceptually and computationally) because it had been presumed previously that the vastly more complicated many-electron wave function was essential for this purpose. In this talk, I present a biographical sketch of Kohn focusing on his highly unusual educational experiences and the events in his professional career which led him to create DFT. A coda explains how the chemists came to award "their" Nobel prize to a card-carrying physicist.

Monday, January 26, 2015, at 3:00 pm

SERC 110A

Refreshments served at 2:45