

Electronic Structure Theory: Yesterday, Today and Tomorrow

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Understanding the vast array of phenomena exhibited by the many-body system of interacting electrons in matter is one of the great challenges of physics. Within a few years after the advent of quantum mechanics, there was basic understanding of metals, insulators and semiconductors. However, quantitative predictions had to await computational power and new developments in theory, most importantly density functional theory (DFT) in the 1960's. New algorithms, notably the Car-Parrinello method in 1980's, have brought the field to the point where it is an essential part of modern materials research.

Today new many-body methods and computational algorithms are being developed. The challenge is to create the capability to make possible robust predictions for properties and new phenomena, illustrated by examples of recent work on nanostructures, metal-insulator transitions, superconductivity, biological systems, and other areas in physics, chemistry, and materials science.