Building on the Successes of Electronic Structure Theory

Richard M. Martin

Department of Physics University of Illinois 1110 W. Green St. Urbana, IL 61801 USA

Understanding of electronic structure of materials has come a long way in the 80 years since 1924 when Prince Louis de Broglie deposited his thesis. From the start electrons have played a key role in the development of quantum theory, and within a few years quantum mechanics provided the underpinnings of present understanding of metals, insulators and semiconductors. Today the field is at a momentous stage, with new algorithms and computational methods, and rapid advances in basic theory. In the 40 years since the advent of density functional theory and the 20 years since the landmark Car-Parrinello paper, the work of many people have brought the field to the point where properties of materials can now be determined directly from the fundamental equations for the electrons [1]. The methods have become standard tools - an essential part of modern materials research. At the same time there have been important developments in many-body theory and methods to treat excitations of correlated, interacting electrons.

This talk is oriented toward the future and the greatest challenges, which are to understand the vast array of phenomena exhibited by the many-body system of interacting electrons in matter. At this point in time there is the opportunity to build upon recent successes to create new approaches that will make possible robust predictions for new phenomena and materials, complex systems, nanostructures, activity of large molecules in solution, magnetism, metal-insulator transitions, transport, and many other areas. Specific examples of recent work show the power of combined independent-particle and many-body methods to provide new predictive capabilities and new insights into important problems in physics, chemistry, and materials science.

[1] An exposition of the basic theory and methods along with extensive references and examples of recent work can be found in "Electronic Structure: Basic theory and practical methods," R. M. Martin, Cambridge University Press (2004), and on-line at `http://ElectronicStructuer.org`.