TSF12-2012-000008

Abstract for an Invited Paper
for the TSF12 Meeting of
the American Physical Society

Answering Dirac's Challenge: Practical Quantum Mechanics for Materials[1]

JAMES CHELIKOWSKY, University of Texas at Austin

Over eight decades ago, after the invention of quantum mechanics, P. A. M. Dirac made the following observation: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems..." The creation of "approximate practical methods" in response to Dirac's challenge has included the one electron picture, density functional theory and the pseudopotential concept. The combination of such methods in conjunction with contemporary computational platforms and new algorithms offer the possibility of predicting properties of materials solely on the basis of the atomic species present. I will give an overview of progress in this field with an emphasis on materials at the nanoscale.

[1]Support from the DOE and NSF is acknowledged.