Beyond Nostalgia: Electronic Structure Concepts for the 21st Century

J. C. Phillips

Dept. of Physics and Astronomy, Rutgers University, Piscataway, N. J., 08854-8019

Abstract

Some 50 years ago, when Len Kleinman and I were helping to lay the foundations for modern self-consistent field calculations, probably the most important issue was the failure at that time of almost all first-principles calculations to yield agreement with experiments, even in the simple cases of elements like Al, Si, and Ge. Because the agreement was so poor, semi-empirical pseudopotential theory (**T**ransparent, **R**eliable, and **T**ransferable) was invented, and it immediately yielded excellent agreement with (and in fact helped to discover) a very large number of band-structure features that had previously been considered beyond the reach of calculation. Today there are reliable, user-friendly self-consistent field programs that virtually guarantee results that are quite close to experiment, even for multiferroic compounds, providing those compounds are crystalline or are composed of small clusters, so what is left to be done? I will discuss this question in the context of ceramic superconductors, where a semiempirical phenomenology, analogous to pseudopotentials for simple elements, and equally successful, has recently appeared, after two decades of total failure by hundreds of alternative theories, including those proposed by upwards of 10 Nobel laureate theorists. The challenge is to translate these successful semiempirical ideas into first-principles models, bearing in mind that the typical quaternary ceramic superconductor has ~ 10 atoms/cell, and these include oxygen, Cu and alkaline and rare earths, all elements which even separately pose delicate problems. BTW: conventional self-consistent field calculations predict that these materials, because their conduction electron density is much lower than that of the alkali metals, should not be superconductive even at 0K, much less at the attained values of 150K.