



Jim

Chelikowsky

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September 29, 4:30 p.m.

Hale Library, Hemisphere Room

Kansas State University

Addressing Dirac's Challenge: Practical Quantum Mechanics to Predict the Properties of Materials

Chelikowsky, a 1970 graduate of K-State in Physics will discuss how after the invention of quantum mechanics, P. A. M. Dirac observed "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 from knowledge of the atomic species present. I will give an overview of progress in this field with an emphasis on materials at the nanoscale.

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