Addressing Dirac's Challenge: Practical Quantum Mechanics for The Discovery and Design of Advanced Materials

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Abstract: Shortly after the invention of quantum mechanics, the famous physicist P. A. M. Dirac wrote the following: "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 ..." (Proceedings of the Royal Society of London. Series A 123, 714 (1929)). Dirac's call to develop practical methods for applying quantum mechanics to materials is one of the "grand challenges" in physics. A resolution of this challenge would allow one to use the laws of quantum mechanics to predict properties of complex materials such as catalysts, ferroelectrics, thermoelectrics, and photocells. The complexity of the laws of quantum mechanics arises from several sources. The probabilistic nature of the electron does not allow one to specify its position in space, only the probability of finding it at a particular point. This increases enormously the degrees of freedom to be specified compared with classical systems and is compounded by the number of interactions present, even for a modestly sized system. Another serious part of the problem is the numerical precision required for a realistic solution. The energy difference between an atom in isolation and the same atom in a molecule is a very small fraction of the total energy of the atom. In short, quantum equations are complex, carry numerous degrees of freedom, and must be solved to a high degree of precision. Our challenge will be to write computer codes capable of describing systems with thousands of atoms by implementing new algorithms and creating numerically efficient solutions using high-performance computing platforms.