Awardee: **James R. Chelikowsky, Professor, Physics**

Research Award Title: Addressing Dirac's Challenge: Practical Quantum Mechanics for the Discovery and Design of Advanced Materials

Research Summary

Our work this past year has focused on the development of practical methods for applying quantum mechanics to complex systems. The development of such methods is a “grand challenge” in materials physics. A resolution of this challenge would allow one to discover, design and understanding advanced materials without experiment, instead using the laws of quantum mechanics and high performance computational platforms.

The complexity of the laws of quantum mechanics arises from several sources and serves as the heart of the challenge. Specifically, 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 enormously increases the degrees of freedom to be specified compared to classical systems and is compounded by the quantum nature of the electron-electron interactions present, even for a modest sized system. Consider that the number of molecules in a glass of water is comparable to the number of stars in the known universe. Compounding 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 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 precision.

We have worked on new algorithms to solve the Kohn-Sham equation. Walter Kohn received the 1998 Nobel Prize in Chemistry for developing “density functional theory," which uses the electron density to construct an effective one-electron theory. The combination of pseudopotentials and density functional theory results in the Kohn-Sham eigenvalue equation. The Kohn-Sham equation yields information on the energetic and spatial distributions of the electronic states of molecules, clusters, liquids and solids across a wide range of length scales. Using this information, one can predict materials properties such as phase stabilities—and optical, dielectric, and magnetic response functions without resort to experiment.

In our previous work, we considered a subspace filter that yielded the eigenvalue space below some maximum eigenvalue. While notably expediting the eigensolution problem, there remain two serious bottlenecks, which limit the ultimate system size. One bottleneck centers on a Rayleigh-Ritz step that requires a solution of a dense matrix set by the size of the number of eigenvalues. For example, if we wish to solve for 20,000 eigen states, we need to solve for all the states in a 20,000 x 20,000 matrix. This step can be partially addressed by available solver, but ultimately this bottleneck limits the size of the system we want to consider. The second bottleneck centers on communication issues in the matrix-vector multiplications of the filter process.