To whom it may concern

Several postdoctoral positions in electronic-structure modeling with Professor Barry Dunietz at Kent State University are available beginning as soon as July 1, 2012. The appointments are in the general areas of computational chemistry and condensed matter. *Ab initio* modeling techniques of material properties at the interface of molecular and bulk systems will be developed and implemented. Relationships of the optical, electronic, and mechanical properties to functionality of the materials will be investigated. The computational modeling research will be pursued in collaborations with experimental and other computational focused groups and the energy frontier research center, the Center for Solar and Thermal Energy Conversion (CSTEC).

The current focus of the electronic structure research is on electron transport through molecular scale bridges and on thermoelectric and photovoltaic energy conversion systems. The specific projects will be determined following the interests of the successful candidates. Some examples of research topics include:

- Electron transport and thermoelectric properties of molecular bridges
- Real space expansions of electron transport models
- Multiscale modeling of transfer processes in organic photovoltaic systems
- Electron dynamics and spectroscopy of molecular bridges

In addition, a variety of systems with biological importance or material science relevance will be considered. Examples include proton transfer studies, enzyme functionality, conducting polymers, optoelectronic materials and liquid crystals.

Applicants with strong background in physics, chemistry, material science or related fields are encouraged to apply. Computational research experience in one or more of the following areas is an advantage: Time dependent DFT methodology, density functionals design, Green’s function formalism, many body methodologies, condensed phase, energy and electron transfer, molecular bridges and nanoscale science.

Applications including a CV, list of publications and suggested letter writers (previous advisers or collaborators) should be sent by email to bdunietz ‘at’ kent.edu. Abstract of research results and reprints of up to two most important papers should be attached to the application. The position is for one year with possible extension to two years. Review of applicants will begin immediately and will continue until all positions are filled.