

POST-DOCTORAL OPPORTUNITIES

Improved Quantum Simulation Methods for Warm Dense Matter

Four well-qualified, energetic post-doctoral associates are sought for this exciting new project. The team will be developing finite-temperature (free-energy) orbital-free density functional theory for first-principles simulations of Warm Dense Matter (WDM).

WDM systems exist in a temperature/density regime such that a variety of mutually interacting charged and neutral species coexist, typically at solid-phase densities with temperatures in the roughly 10 eV range. WDM occurs in situations ranging from planetary science (e.g. the interiors of the jovian planets) to thermonuclear energy production. WDM is an exciting challenge to theory because this state of matter is not well represented by models applicable in the limit of either high or low temperature or density. Our approach is to use constraint-based, free-energy density-functional theory in an orbital-free framework. We will be developing constraints on kinetic energy, non-interacting entropy, and exchange-correlation functionals, building new approximate functionals, programming, testing, and using them. We will build from existing knowledge of orbital-free theory in both the high-temperature and zero-T limits.

We seek four team members who can contribute creatively. Strong candidates will have relevant knowledge and skills, in most cases including one or more of: density functional theory; modeling and simulation; plasma physics; statistical mechanics; computational methods. Candidates must have a Ph.D. or D.Sc. (or clear equivalent) in computational and/or theoretical Physics or in theoretical and computational chemistry or in a functionally equivalent discipline (e.g. Materials Science) or have fulfilled **all** requirements for such a degree with the award of the degree pending.

The project environment will be that of a collaborative team. Post-doctoral associates can expect to work with two or more of the senior participants (S. B. Trickey, PI; J. W. Dufty, F. E. Harris, and K. Runge, co-PI's.)

Funding, under the U.S. Dept. of Energy Theory, Modeling, and Simulation program, is expected to be available September 1, 2009. Initial appointments will be for 12 months, renewable by mutual agreement. Qualified, interested persons should send their Curriculum Vitae (in PDF please) and provide names and contact information of three professional references to Prof. Sam Trickey, trickey@qtp.ufl.edu. If accommodation due to disability is needed, call 352-392-4621 or (TDD) 800-955-8771. UF is an equal opportunity employer.