

13 May 2020

NEW POST-DOCTORAL POSITION AVAILABLE

A new post-doctoral position is available beginning June 1, 2020 in the group of Sam Trickey (Physics and QTP, Univ. of Florida) in funded collaboration with Antonio Cancio (Dept. of Physics and Astronomy, Ball State Univ.).

The focus is development and efficient application of accurate density functional approximations that are orbital-free. This includes "de-orbitalizing" of high-rung functionals such as metaGGAs and constraint-based construction of new functionals from scratch. Project goals are

- (1) to cap the scale-up of computational costs for ab initio molecular dynamics simulations of complex materials, by eliminating explicit dependence upon Kohn-Sham (KS) orbitals in exchange-correlation (XC) functionals.
- (2) to develop true KS quantities with mGGA quality or better, rather than the generalized KS solutions usually done today with meta-GGAs;
- (3) to push the utility of constraint-based approximate XC functionals dependent only on the electron density and its derivatives as far as feasible.

Tasks undertaken by the Post-doc may include: discovery of constraints and other basic properties of the kinetic and XC energies, key targets for de-orbitalization; development of new functionals from a fundamental, constraint-based approach; address of technical challenges in implementing such functionals (e.g., long-standing issues of stability when density-Laplacians are used); implementation of new functionals in major codes such as VASP, QuantumEspresso, NWChem, and applications.

A Ph.D. (or equivalent) in physics, materials science, chemistry, or closely related discipline is required. Experience in development of approximate functionals is highly desirable. Experience in coding new functionals in large complex codes (e.g. QuantumEspresso, VASP, etc.) also is relevant. (Experience in ordinary use of such standard codes is *NOT* sufficient.)

Close collaboration with both the PI and the senior collaborator is an intrinsic opportunity. That includes virtual and in-person meetings and interaction with the graduate student funded on the project at Ball State. For further detail see <http://www.qtp.ufl.edu/ofdft> and <https://www.bsu.edu/academics/collegesanddepartments/physics-astronomy/about/faculty-staff-directory/cancioantonio>

Funding is assured for the first year from our new NSF grant, with renewal subject to satisfactory evaluation and mutual agreement. Salary will be commensurate with relevant experience and accomplishments.

Applicants should provide Prof. Trickey ([trickey at qtp.ufl.edu](mailto:trickey@qtp.ufl.edu)) the following:

- [A] a cover letter that addresses clearly but briefly how your experience matches the areas of experience listed above;
- [B] your curriculum vitae (including publication list and your contact information);
- [C] a statement of your immigration status (if not a US citizen or permanent resident);
- [D] the names and contact information for three references;
- [E] earliest feasible start date

All candidates for employment at Univ. of Florida are subject to a pre-employment screening which includes a review of criminal records, reference checks, and verification of education.

The final candidate will be required to provide an official transcript to the hiring department upon hire. A transcript will not be considered "official" if a designation of "Issued to Student" is visible. Degrees earned from an educational institution outside of the United States require evaluation by a professional credentialing service provider approved by the National Association of Credential Evaluation Services (NACES), which can be found at <http://www.naces.org/>.

The University of Florida is an equal opportunity institution dedicated to building a broadly diverse and inclusive faculty and staff. Searches are conducted in accordance with Florida's Sunshine Law. The Physics Department particularly welcomes applicants who can contribute to a diverse and inclusive environment through their scholarship, teaching, mentoring, and professional service. The university and greater Gainesville communities enjoy a diversity of cultural events, restaurants, year-round outdoor recreational activities, and social opportunities. If an accommodation due to disability is needed to apply for this position, please call (352) 392-2477 or the Florida Relay System at (800) 955-8771 (TDD).