Department: Physics and Astrononmy
Position Title: Nanoscience Graduate Assistant
Supervisor: Antonio Cancio
Supervisor Title: Assistant Professor of Physics

Position Function Statement

This assistantship is a continuation of a National Science Foundation funded project to develop and implement novel ideas for improving density functional theory, the theoretical foundation for the computational simulation of materials at the atomistic level. It will allow the recipient to pursue a full-time course of study at Ball State leading to the Master of Science degree in physics. The student will have the opportunity to participate in cutting-edge research in electronic structure theory, to interact with faculty and students in the department's Center for Computational Nanoscience, and the opportunity to present results of the work at national meetings and in peer-reviewed journals.

Position Activities

The successful applicant will participate in one or more of the following activities:

1. Learn the fundamental principles of density functional theory and the techniques of electronic structure calculations.
2. Build tools to analyze and visualize numerical data from Monte Carlo and other simulations of electronic structure.
3. Assist in the design, implementation and testing of new models for density functional theory.
4. Perform electronic structure calculations of various classes of solids and molecules and calculate structural properties such as cohesive energies, lattice constants and bulk moduli, using standard electronic structure software such as ABINIT and Gaussian.
5. Perform electronic structure calculations of metallic surfaces and model related magnetic properties.
6. Develop Unix scripts to automate testing procedures.
7. Create and maintain computer notebook of results and perform statistical data analysis on them.
8. Present results in regional and national meetings.
9. Assist in the summarizing of results for peer-reviewed journals.

10. Prepare educational materials for use by the Physics department in solid-state physics and related classes.

11. Interact and cooperate with faculty and students of Center of Computational Nanoscience at Ball State.

Minimum Required Qualifications

A bachelor's degree in Physics or a related field such as Chemistry or Materials Science is required. The applicant must have met the conditions for admission in to the Ball State University Graduate School, including maintaining a GPA of 2.75 or higher. The applicant should have taken, or plan to take, a course in solid state physics at the undergraduate level or higher and a course in introductory computer science. The applicant should have basic computer and internet skills for performing scientific research, such as the use of Excel, Matlab, or Mathematica, have good organizational and note-taking skills and effective written and oral communication skills.

Additional Preferred Qualifications

A GPA of 2.90 or higher is preferred. Experience working in a Unix operating environment is desirable, and knowledge of a programming or scripting language such as Fortran, C/C++, Python.

Job Context

The applicant must be able to work for long periods of time at a computer performing tasks such as running simulation code, data analysis and graphing, data file management, creating presentations, with occasional participation in collaborative activities, group meetings, training sessions etc. The successful student will be organized, conscientious in paying attention to details in performing research and able to work towards long-term goals without close supervision.

Supervision Received

The applicant will work under varying degrees of supervision. Some activities, such as initial training will be closely supervised; student is expected eventually to work with only moderate to indirect supervision.

Supervision Provided

The applicant will be required to provide training in running simulation codes and run scripts to new members of the project.