



Midwest Integrated Center
for Computational Materials

The Midwest integrated center for computational materials (MICCoM, <http://miccom-center.org>) is looking for two postdoctoral researchers to join the development teams located at Argonne National Laboratory and University of California, Davis.

This position is sponsored by the U.S. Department of Energy within the context of a broad project aimed at enabling exascale calculations of materials properties. The postdoctoral researchers will primarily work with Prof. G. Galli, Prof. F. Gygi and Dr. M. Govoni, and with a team of 10+ PhDs/postdocs contributing to the development of codes currently supported by MICCoM (<http://miccom-center.org/software.html>).

Excellent candidates are sought with experience in the development of complex scientific software architectures to support the development and deployment of MICCoM codes on pre- and exascale architectures. The candidate will port to GPUs the software for electronic structure (WEST, <http://west-code.org>) and/or molecular dynamics (Qbox, <http://qboxcode.org>) calculations.

The salary is competitive and commensurate with experience. The position at Argonne National Laboratory may lead to subsequent employment in a software scientist role, depending on performance and mutual interest.

Major duties and responsibilities:

- Algorithmic development for GPU programming
- Code development and optimization for high performance architectures

Position Requirements:

- Experience with GPU programming

Skills and experience:

- Proficient in C++ and/or Fortran
- Knowledge of Python
- Experience in algorithm optimization and parallel programming (MPI, OpenMP)
- Experience in professional software development (including version control systems, issue trackers, unit testing, continuous integration)
- Experience with debugging/profiling tools
- Excellent communication skills
- Ability to work in a team

A scientific background in physical, chemical-physical or engineering sciences, and an expertise in molecular dynamics and/or in electronic structure codes is preferred. Basic knowledge of the internal functioning of MICCoM codes would be an advantage but is not required. Typical candidates will be independent and motivated individuals with MSc or PhD in Materials Science, Computer Science, Physics, Chemistry or Chemical Engineering or comparable skills and experience.

For inquiries and applications, please contact Giulia Galli (gagalli@uchicago.edu), Marco Govoni (mgovoni@anl.gov) and Francois Gygi (fgygi@ucdavis.edu).