Postdoctoral Appointee - Functional Materials for Energy Conversion -- Early Science Program on Theta at Argonne National Laboratory (ANL)

Candidate will work on an ALCF Early Science Program (ESP) project http://www.alcf.anl.gov/articles/alcf-selects-projects-theta-early-science program targeting first principles simulations of functional materials for energy conversion on ANL forthcoming Theta supercomputer. The project PI is Prof. G. Galli (University of Chicago). Ideal candidates will have scientific expertise in electronic structure methods, knowledge of high performance computing (compilers, libraries, hardware), and be active participants in the research.

Computational methods will include ab initio molecular dynamics with semi-local and hybrid functionals and many-body perturbation theory, using the Qbox (http://qboxcode.org/) and WEST (http://www.west-code.org/) codes developed at the University of California Davis and at the University of Chicago, respectively. This postdoc will draw on knowledge of electronic structure and high performance computational (HPC) science to prepare and optimize codes for the >8 petaFLOPS Cray/Intel system based on the 2nd Generation Intel Xeon Phi processor (Knights Landing: KNL). Performance tools will be used to identify bottlenecks in simulations (load imbalances, I/O problems, memory constraints, etc.).

The activity will be supervised by Prof. G. Galli (UChicago) and Prof. F. Gygi (UC Davis), and will be carried out in collaboration with Dr. M.Govoni (ANL). The postdoc will also work closely in collaboration with multi-disciplinary science project teams including the project PI and team members, ALCF staff, and Cray/Intel staff. This two-year position is based at the ALCF, but the postdoc will travel to home institutions of project investigators as appropriate for close collaboration.