

Title: Predicting Catalysis at Oxide Nano-Particles
Type: Postdoc
Awardee: Kiril Tsemehkman
Mentors: Hannes Jonsson – UW; Eric Bylaska - PNNL
Abstract: We will implement improvements to the density functional theory approach in order to achieve proper theoretical description of band gaps and spin states of transition metal oxide surfaces. This methodology will be implemented in the parallel plane-wave based module of NWChem and it will be applied to the study of molecular binding and reaction at the iron and nickel oxide surfaces. The three applicants have already collaborated for several years on this project and a first version of the code is already a working part of the NWChem package. The requested funds will pay for application calculations related to the catalysis of nanoscale oxide particles, in direct connection with an ongoing nanotechnology project at PNNL directed by Dr. Baer, as well as for the continuation of the development work. The requested funds will provide salary for the post-doc, Kiril Tsemehkman, one of the three applicants.