Travel Report for JUSTIPEN Hokkaido Workshop

William A. Shelton
Computational Chemical Sciences Group
Oak Ridge National Laboratory

It was an honor to be invited to present my work on the density functional theory, multiple scattering based dynamical cluster approximation (specialization of dynamic mean field theory) for treating disordered systems beyond mean field theory and on the development of highly parallel Multiple scattering based electronic structure method that scales linearly with increasing system size. I enjoyed extensive conversations with our Japanese colleagues (especially Prof. Shimizu and Prof. Itagaki) on my work on disordered systems and on the screening techniques used in my electronic structure code. I also had discussions with Prof. James Vary, Prof. Shalom Shlomo and Dr. P. Maris on the aforementioned topics and on multiwavelets and non-linear Broyden based optimization techniques. I also enjoyed extensive discussions on numerical methods and parallel computational methods with post-doctoral fellows, junior faculty and graduate students. The enthusiasm for developing interdisciplinary collaborations is inspiring.

I would also like to thank Prof. Itagaki and Mrs. Yoshida and their staff for their exceptional hospitality.