**Investigation of high entropy alloys with LSMS method**

Xianglin Liu, Markus Eisenbach, Yang Wang, G. Malcolm Stocks

Oak Ridge National Laboratory

[liux4@ornl.gov](mailto:liux4@ornl.gov)

**Abstract**

High entropy alloys (HEA) are a class of materials that demonstrate many promising mechanical properties. Due to the complex chemical environment, a proper treatment of HEA typically requires a large supercell, which is expensive for traditional DFT methods due the cubic scaling behavior. In this work, we investigate a range of HEAs using the locally self-consistent multiple scattering (LSMS) method, which scales linearly with respect to the number of atoms. Using supercell of up to 1280 atoms, we calculate the lattice constants and bulk modulus of both FCC and BCC HEAs. Moreover, we investigate the chemical fluctuations in HEAs by examining both the variance of total energies and the local charge transfer profile, which gives insight to the construction of theoretical models to fully incorporate the effects of chemical fluctuation.