The reverse Monte-Carlo code is a simple code based on the Ising model which can predict the most stable crystal structure at any temperature. It is kind of an inverse problem where the atoms at all possible locations in a crystal is considered. Atoms are taken out at random from their lattice sites which gives a certain energy to the crystal. If the difference in the energy of minimum energy lattice and the energy of the current lattice comes out to be lesser than the Boltzmann criteria then we make the present lattice as the minimum energy lattice. We keep the randomization process of creating different lattices and finding its minimum energy long enough. We obtain the minimum energy lattice once the process reaches equilibrium. The energy profile and structure factor of the lattices can be compared with DFT or experimental results to determine the stable lattice.

The Monte-Carlo code takes the structure information (geo) in .bgf format. It requires a energy minimization setting (CONTROL), force field (ffield), a submission script (run.sh). We ran the particular code in conjunction with the ADF platform where the energy minimization of the lattice is performed. It can also run in any other platform like LAMMPS or standalone versions. We used ReaxFF force field for the minimization process.