**Monte-Carlo algorithm for calculation of configurational energy density of states, application to lithium ion conductor LLTO**

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In this work a Monte-Carlo algorithm is presented that uses random sets along with Wang and Landau importance sampling to calculate the configurational energy density of states. The algorithm is referred to as BLENDER (Blend Each New Density Each Round). The algorithm is natural to parallelize and is developed from a self consistent approach. The algorithm is also naturally suited for lattice type problems. The algorithm is tested with the 2-d Ising model up to size of 256X256. The bench marks with the 2-d Ising model show the algorithm is promising. The main goal of developing this algorithm was the computation of partition functions of materials with disordered sub lattices. To further test the algorithm it is trialed with a 90atom supercell of disordered tetragonal Li0.5La0.5TiO3 (LLTO). These calculations were performed at the level of GGA-PBE density functional theory. Although the 90atom supercell restricts the modeling of the Li La disorder , the evaluation of the configurational energy density of states with the developed algorithm still gives insights into the physics of the configurational disorder for this system. Understanding the Li La disorder in LLTO is important for on going research in modeling LLTO-LMO and Li-LLTO-LMO interfaces.