The structure of manganese lithium borate-based glass was studied by using molecular dynamic (MD) simulation. In this work, a glass system of 0.2MnO2 – 0.8(Li2-2B2O3) was introduced. DL_POLY MD package[1] based on Buckingham potential parameter[2,3,4] was employed to calculate structure of this glasses. The ten pair radial distribution functions of this glass were obtained from the MD simulation. To understanding this glass structure, MD-EXAFS result which came from FEFF8.2 package[5] was compare with EXAFS spectrum at Mn K–edge of this glass. Consequently, a good agreement between calculated and measured EXAFS data was obtained leading to a fully address of local structures of this glassy materials with a mean Mn-O coordination network of 3.01(2).

Keywords: Manganese Lithium Borate Glass, Molecular Dynamics Simulation, EXAFS.