Towards reliable structural information of multicomponent glass systems

Christoph Scherer, Martin Hetz, Friederike Schmid

The final goal of this work is to find the best way of generating reliable glass structures on the computer. Here, the model glass formers SiO_2 and B_2O_3 are examined and the glass structures are generated in the following way. Configurations of a few hundred atoms are equilibrated at high temperature, well above the glass transition temperature, by means of classical MD simulation. After a quench down to 0K, they are structurally relaxed to the next (local) minimum by means of an ab inito (DFT) calculation. The final structure and vibrational properties are compared to experimental results from neutron scattering. In case of B_2O_3, the dependence of the glass structure on the classical force field is examined and compared to a full ab initio quench. Therefore, a set of model force fields is generated by means of a structural fitting procedure to an ab initio trajectory.