Glass structure with well defined thermal history and glassy dynamic

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Glasses have a huge range of applications, however, they are still theoretically not well understood. Also experimental access to the structure of glasses is limited. This motivates the study of glass systems by means of computer simulations. In this work a set of glass structures with well defined thermal history is generated on the computer. In one approach, glass structures are created by gradually cooling down a set of 100-200 atoms by means of a molecular dynamics simulation as long as the system still can be equilibrated in reasonable simulation time with a subsequent quench down to room temperature. In another approach, the set of atoms is linearly cooled down to room temperature. These configurations are used as a starting point for a quantum-mechanical relaxation by means of density functional theory. Then, structural quantities are compared before and after the relaxation and to experimental results. Especially, the vibrational spectrum is of interest, as thereof thermodynamical quantities, as the temperature dependent specific heat, can obtained. First successful tests on the model glass former SiO2 are presented.