Classical Non-Equilibrium Molecular Dynamics in SiO_2 systems

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SiO_2-based materials are of a great importance due to their important role in different fields, as biomedicine,[1] optics,[2] photonics,[3] and electronics[4]. Moreover, one of the most important silica polymorphs, namely alpha-quartz, is a very common mineral and it is stable down to 100-km depth from the surface.[5] This makes this material a very interesting object of study in the geoscientific context. Several efforts have been reported in the literature in order to shed light into the nano-scale properties of these materials. A very powerful tool that can be used with this purpose is classical Molecular Dynamics, which allows the study of atomic interactions at a reasonable computational cost. Non-Equilibrium Molecular Dynamics simulations will be performed to analyse the propagation of an artificial perturbation in silica systems. This propagation will be analysed by means of different metrics and the corresponding results will be compared.

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