Screening dependence of the dynamical and structural properties of BKS silica

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Résumé en anglais	Molecular dynamics simulations of amorphous silica are carried out on a large temperature range using a modified version of the BKS inter-atomic potential. We investigate the dependence on the screening procedure of the structural and dynamical properties of amorphous silica. We show that an increased screening of the electrostatic interaction leads to a decrease of the diffusion constants and then to better agreement with experimental data, while structural properties are unchanged. We show that the Arrhenius dependence of the diffusion constants may be reproduced in this case up to a temperature of 4000 K with activation energies very similar to the experimental data.
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[4] http://okina.univ-angers.fr/publications?f[keyword]=14254
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