Transient self-organisation of supercooled water confined inside nano-porous materials

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Résumé en anglais	Large-scale molecular dynamics simulations are used to investigate the structural and dynamical modifications of supercooled water when confined inside an hydrophilic nanopore. We then investigate the evolution of the auto-organisation of the most and the least mobile molecules (dynamical heterogeneity and string-like cooperative motions) when supercooled water is confined. Our calculations use the recent TIP5P intermolecular potential for water. We observe a strong slowing down of the dynamical properties when the liquid is confined, although the liquid structure is found to remain unchanged in the centre of the pore when corrected from the pore geometry. We then study cooperative motions inside supercooled confined water in comparison with bulk water. We observe strong modifications of the cooperative motions when the liquid is confined. We observe that dynamical heterogeneities and the associated correlation lengths are strongly increased as well as string-like motions in the confined liquid. This result, which is in opposition with the expected limitation of the correlation length by the confinement procedure, may explain (or be explained by) the slowing down of the dynamics. However the comparison of the dynamical heterogeneities at constant diffusion coefficient shows that the slowing down of the dynamics is not sufficient to explain the increase of the correlation lengths.
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