Molecular dynamics simulation of silver nanoparticles in a europium doped sodosilicate glass

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Résumé en anglais	Molecular dynamics simulation is applied to an europium doped sodosilicate glass containing silver [(Na–Ag)2O–SiO2–Eu2O3]. The silver is implanted in substitution of Na, simulating an ionic exchange. For ionic interactions a modified Born–Mayer–Huggins potential was employed. For the Ag–Ag interaction, a Lennard-Jones (LJ) potential is applied, while for the Eu–Ag interaction, a modified LJ potential is introduced. The particle size increases with the annealing treatment and follows a lognormal law. After 75 ps the average particle size reaches 5.8 atoms (4.8 for Ag and 1.0 for Eu), and it is found that the europium is preferentially situated on these nanoclusters.
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