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Structure of charge trapping in cerium-doped aluminophosphate and phosphosilicate glasses: combining molecular dynamics simulations and *ab initio* DFT calculations LEOPOLD KOKOU, YUN LI, JINCHENG DU, University of North Texas, MSE TEAM — Cerium doping glasses find wide applications in optical and photonic devices. Both Ce^{3+} and Ce^{4+} can be present in oxide glasses, and their ratio depends on the glass composition, heat history and melting environment. In either oxidation state, the environments of cerium ions are important to the optical absorption and emission properties. In this paper, we present classical molecular dynamic simulations of cerium-containing aluminosilicate and phosphosilicate glasses using newly developed potential models containing cerium ions. The local environments around Ce^{3+} and Ce^{4+} are studied, and the bond length and coordination of cerium ions are determined. Small samples of the glasses are simulated using MD and then further relaxed with Density Functional Theory (DFT) calculations. Comparison of the structure of glasses from MD and after DFT relaxation is made, and the two are found to be in reasonable agreement. It is found that Ce^{3+} has a longer bond distance and higher coordination number of oxygen. Most interestingly, cerium ions are found to be preferentially coordinated by phosphorus ions in the second coordination shell in the glasses.

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