
He incorporation in nuclear waste glass: Insight from Density functional theory

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Abstract

Radioactive fission products confined in nuclear waste glass decays in a variety of pathways. Alpha, beta and gamma produce recoils and electronic effects, which involves electronic excitation. In addition, it is known that the presence of alpha particles can create gaseous species that can nucleate to form bubbles. To unveil the effect brought to the structure of nuclear waste glass by the presence of He, density functional theory is used to analyze the synergetic and the topology of interstitial sites in the International Simple Glass (ISG). Four sets of calculations were conducted in which the number of He atoms was increased gradually in the glass network, The size of the interstitial sites and their formation energy are measured and compared to available data in the literature. The electronic density of states and glass structure were used to determine the bonding nature of He atoms.

Keywords: DFT, Nuclear waste management, Bubble formation, Molecular Dynamics, International Simple Glass

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