Structural, elastic, vibrational, and electronic properties of amorphous Al_2O_3 from *ab-initio* calculations[1]

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First principles molecular dynamics calculations of structural, elastic, vibrational, and electronic properties of amorphous Al_2O_3, in a system consisting of a supercell of 80 atoms is reported. A detailed analysis of the interatomic correlations allows us to conclude that the short-range order is mainly composed by AlO_4 tetrahedra, but, in contrast with previous results, also an important number of AlO_6 octahedra and AlO_5 units are present. The vibrational density of states presents two frequency bands, related to bond-bending and bond-stretching modes. It also shows other recognizable features present in similar amorphous oxides. We present also calculation of elastic properties (bulk modulus and shear modulus). The calculated electronic structure of the material, including total and partial electronic density of states, charge distribution, electron localization function (ELF) and the ionicity for each species, gives evidence of correlation between the ionicity and the coordination for each Al atom. A discussion with respect to earlier molecular dynamic simulations and experimental results will be presented.

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