Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra

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We analyse the principal vibrational spectra of vitreous GeO$_2$ and derive therefrom structural properties referring to length scales beyond the basic tetrahedral unit. We generate a model structure which yields a neutron structure factor in accord with experiment. The inelastic-neutron, the infrared, and the Raman spectra, calculated within a density-functional approach, also agree with respective experimental spectra. The accord for the Raman spectrum supports a Ge-O-Ge angle distribution centered at 135°. The Raman feature $X_2$ is found to result from vibrations in three-membered rings, and therefore constitutes a distinctive characteristic of the medium-range structure.

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