

Abstract Submitted
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Medium-Range Structural Properties of Vitreous Germania Obtained through First-Principles Analysis of Vibrational Spectra LUIGI GIACOMAZZI, PAOLO UMARI, ALFREDO PASQUARELLO, Ecole Polytechnique Fédérale de Lausanne (EPFL), Institute of Theoretical Physics, CH-1015 Lausanne — 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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