



Séminaire – Lundi 11 janvier – 14H00
Salle PMC (05-3029A)

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13H30

THE VIBRATIONAL MODES TREATMENT AND RAMAN ANALYSIS OF VITREOUS SILICA UPON MECHANICAL LOADS AND LASER TREATMENT

We perform a simulation of vitreous silica to calculate the vibrational modes. Partial and total vibrational densities of states are presented. To reveal the structure of the vibrational spectrum, the characteristics of vibrational modes in different frequency ranges are investigated using a mode-projection approach at different symmetries. The sensitivity to mechanical loads and multi-/single-pulse IR laser irradiation, especially, an irreversible densification is explored. We consider the main experimental bands, and relate them to a detailed description of the vibrations. Finally, we compare our Raman and VDOS spectra with experimental ones, and show that Raman investigations provide reliable structural insight.