

Test: F.P. v-DOS of v-SiO₂

- Silica glass model 72 atom (216 vib. Modes)
- Tests carried out using 3x20=60 cores (Intel Xeon E5-2680 v2 2.80 GHz).
- (V-DOS) dynamical matrix calculated by finite differences using the QE v.6.2 cp.x in 2 hours.
- V-DOS calculated using QE ph.x v.6.2 in 5 hours.

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Medium-range structure of vitreous SiO₂ obtained through first-principles investigation of vibrational spectra

1 / 1