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Atomistic study of vibrational properties of γ-Al_2O_3

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We present the vibrational density of states (v-DOS) for γ-Al_2O_3. The calculation has been made using both lattice dynamics by means of empirical potential and by ab-initio methods. In the former case, we use the inter-atomic potential for alumina due to Catlow and the one by Streitz and Mintminre. In the ab-initio calculation, we use Density Functional Perturbation Theory as implemented in the PHONON code of the package Quantum-ESPRESSO. According to our calculations, we can observe that in general the v-DOS range from 0 to 27 THz and has two main bands, one from 0 to 15-20 THz and another from 20 to 27 THz. The low frequency band is related to inter building-blocks vibration, while main contribution to the high frequency band comes from the intra building-blocks vibrations.