Structural Stability and Vibrational analysis of Yttrium oxide from the Bulk to the (n,0) Nanotubes. An ab initio description

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In this work, we report reliable *ab initio* quantum mechanical simulations of a variety of physical properties concerning the Yttrium oxide (Y_2O_3) in different arrangements from the bulk, the monolayer (*h*-Y_2O_3), to the (n,0) single-walled nanotubes in the range from n = 6 to 64. Structural parameters, phonon modes frequencies and intensities are computed via Density functional theory (DFT/B3LYP) level of theory where the trend towards the (*h*-Y_2O_3) monolayer for large nanotube radius is discussed. For the (n,0) Y_2O_3 nanotube family, two sets of IR active phonon modes in the (300–400 cm^{-1}) and (700–00 cm^{-1}) ranges are determined. Both of them tend smoothly with different slope, towards the optical vibrational modes of the *h*-Y_2O_3 layer. Three sets of active phonon bands are obtained in their Raman spectrum. The first one namely A in the in the 0- 100 cm^{-1} range contains two phonon modes, their vibration frequencies tend to zero at very large tube radius and found to be connected to the elastic constant C_{11} and C_{66} of the *h*-Y_2O_3 monolayer as the 1D →2D transition is approached. The second one namely B in 250-400 cm^{-1} range tends to the optical modes of the monolayer. The third set namely C in the 650-800 cm^{-1} rang contains two active modes, their intensities tend to zero in the limit of large nanotube without change in their vibration frequencies.