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Phonons and related spectra in V_2O_5 bulk and monolayer(001)[1]
CHURNA BHANDARI, WALTER R.L. LAMBRECHT, Case Western Reserve University — We study the phonons at the zone center for the layered material V_2O_5 using density functional perturbation theory. The mode frequencies and their calculated infra-red and Raman spectra are shown to be in good agreement with results from literature. We find better agreement with the experiment, using a pseudopotential that treats vanadium semicore states 3s and 3p as bands. We also study the changes between bulk and monolayer using the same method. We find significant changes in some phonon frequencies. In particular, we see the high frequency modes related to bond-stretching between vanadium and vanadyl-oxygen exhibit a blue shift while a few low-frequency modes show a red-shift. The interatomic force constants, separated in their long-range and short range components are used to analyze the origin of these shifts. We find that the blue shifts arise predominantly from a change in the long-range force constants which is due both to the change in dielectric screening and the change in the Born effective charges.

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