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Electronic band structure and phonons in V2O5 CHURNA BHANDARI, WALTER R.L. LAMBRECHT, CWRU — Among the vanadium oxides, V_2O_5 presents special interest as a layered material. As for other layered materials, it is of interest to search for changes in its electronic structure and phonon spectrum in the monolayer modification of this material. For example, reduced screening may modify phonon modes affected by long-range Coulomb interactions. As a preliminary we here present a first-principles study of the bulk electronic band structure and the phonons at the Γ-point. Density functional calculations in the local density approximation were carried out for the electronic band structure and the density functional perturbation method was used for the phonon calculations. We used LDA and norm-conserving pseudopotentials in the abinit code. A group theoretical analysis is used to label the phonon modes. Non-analyticity is included for the LO modes. The band structures are in good agreement with previous work and yield an indirect band gap. Relaxed structural properties are also in good agreement with experiment. Simulated infrared and Raman spectra will be presented. Our results will be compared with experimental and previous theoretical work.

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