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Phonon Softenings and the Mott-spin-Peierls Transition in VO_2
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To explore the driving mechanisms of the metal-insulator transition (MIT) and the structural transition in VO_2, we have investigated phonon dispersions of rutile VO_2 (R-VO_2) in the DFT and the DFT+U (U: Coulomb correlation) band calculations. We have found that the phonon softening instabilities occur in both cases, but the softened phonon mode only in the DFT+U describes properly both the MIT and the structural transition from R-VO_2 to monoclinic VO_2 (M_1-VO_2). The present *ab-initio* phonon dispersion calculations clearly demonstrate that the Coulomb correlation effect plays an essential role of assisting the Peierls transition in R-VO_2 and producing the spin-Peierls ground state in M_1-VO_2.

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