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 cor-
relation 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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Date submitted: 07 Nov 2012

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