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Correlation between charges and phonons in the phase transition of VO_2[1] BIN WANG, Department of Physics and Astronomy, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and ORNL — Interplay among the microscopic degrees of freedom in transition-metal oxides can generate macroscopic quantum phenomena that provide functionality in electronic and photonic devices. Here, we report density functional calculations and molecular dynamics simulations of VO_2, which undergoes a semiconductor-to-metal phase transition accompanied by a monoclinic-to-rutile structural change at 68 ° C. We find that the lattice vibration at the critical temperature generates a metallic state in the monoclinic structure, which may explain the observed metallic intermediate phase in experiments. Moreover, we find that the electron/hole doping strongly couples with the lattice vibration causing collapse of one particular phonon mode and stimulating the structural phase transition. Molecular dynamics simulations show a temperature-dependence of the required carrier density for the phonon collapse, that is, at higher temperature, fewer free carriers are required. We show that the abrupt change of the vibration results from the weakening of the V-V bonds induced by the hole doping.

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Bin Wang
Department of Physics and Astronomy, Vanderbilt University

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