Abstract Submitted
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Plasmonic electron injection drives ultrafast phase transition by catastrophic phonon collapse II: theory[1] BIN WANG, KANNATASSEN APPAVOO, Vanderbilt University, NATHANIEL BRADY, University of Alabama, Birmingham, MINAH SEO, LANL, JOYEETA NAG, Vanderbilt University, ROHIT PRASANKUMAR, LANL, DAVID HILTON, University of Alabama, Birmingham, RICHARD HAGLUND, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University, ORNL — The ultrafast photo-induced phase transition in VO_2 is promising for data storage and sensing applications. Our experimental work (the previous talk) shows that in a Au/VO_2 hybrid nanostructure, electrons excited in the Au photocathode by an ultrafast laser trigger the insulator-to-metal transition in VO_2. Here we report first-principles density-functional calculations showing that the collapse of a 6 THz optical phonon, corresponding to a twisting motion of V atoms, is responsible for the ultrafast phase transition. Above a concentration threshold, we find that injected electrons from Au induce collapse of the VO_2 phonon, which stimulates the monoclinic-to-rutile structural phase transition. We also show that hole-doping can induce the same effect. The abrupt change of the critical phonon results from the weakening of the V-V bonds induced by the combined flux of injected electrons and holes. Thus, our results explain the experimental finding of plasmonic-electron-driven ultrafast phase transition and represent a step towards manipulating the photo-induced phase transition by surface modification.

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