Abstract Submitted for the MAR14 Meeting of The American Physical Society

Hydrogen Dynamics and Metallic Phase Stabilization in VO_2^1 KEITH H. WARNICK, BIN WANG, SOKTRATES T. PANTELIDES, Vanderbilt Univ — Hydrogen doping has been demonstrated to lower the VO₂ semiconductorto-metal phase transition below room temperature. We report the results of DFT calculations that show that metallic phase stabilization is due to the lattice distortion caused by interstitial hydrogen attached to oxygen atoms. We show that doping is energetically favored and that there is a fast diffusion in the monoclinic [100] direction that can facilitate atomic hydrogen uptake through surfaces that expose these channels. However, the dissociation of molecular hydrogen on a monoclinic (100) surface has a 1.6 eV activation barrier that impedes hydrogen association or dissociation at the surface without significantly elevated temperatures. These results emphasize the role of lattice distortion in the VO₂ phase transition and suggest methods to improve the use of hydrogen doping to control the properties of VO₂.

¹This work was supported in part by DTRA grant HDTRA1-10-0047 and by the McMinn Endowment at Vanderbilt University. Calculations were performed on AFRL DSRC computing resources.

Keith H. Warnick Vanderbilt Univ

Date submitted: 13 Nov 2013

Electronic form version 1.4