Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Photoinduced phase transitions in narrow-gap Mott insulators: the case of VO_2[1] ZHUORAN HE, ANDREW MILLIS, Columbia University — The nonequilibrium dynamics of strongly correlated electrons in photoexcited VO_2 is studied using the quantum Boltzmann equation and nonequilibrium Hartree-Fock methods applied to a band structure given by extended density functional theory (DFT+U+V) and realistic dynamical interactions. The initial equilibration of electrons occurs in hundreds of femtoseconds. For physically reasonable parameters, our Hartree-Fock calculation sustains a new metastable M_1 metal phase that is qualitatively consistent with the recent experiment of Morrison et al [1]. The long-term stability of the M_1 metal phase will also be considered. [1] V. R. Morrison, R. P. Chatelain, K. L. Tiwari, A. Hendaoui, A. Bruhács, M. Chaker, and B. J. Siwick, Science 346, 445 (2014).

[1]This work is supported by the Department of Energy under grant number DE-SC0012375.

Zhuoran He
Columbia University

Date submitted: 05 Nov 2015 Electronic form version 1.4